The Coordination Chemistry of "[BP_3]NiX" Platforms: Targeting Low-valent Nickel Sources as Promising Candidates to $L_3Ni{=}E$ and $L_3Ni{\equiv}E$ Linkages

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Supporting Information

General X-ray diffraction experimental information

Crystals were mounted on a glass fiber with Paratone-N oil. Crystallographic data were collected on a Bruker P4 diffractometer (0.71073 Å MoKα) with a CCD area detector. Data were collected using the Bruker SMART program, collecting ω scans at 5 ϕ settings. Data reduction was performed using Bruker SAINT v6.2. Structure solution and structure refinement were performed using SHELXS-97 (Sheldrick, 1990) and SHELXL-97 (Sheldrick, 1997).

Refinement of F^2 against ALL reflections. The weighted R-factor (*w*R) and goodness of fit (S) are based on F^2, conventional R-factors (R) are based on F, with F set to zero for negative F^2. The threshold expression of $F^2 > 2\sigma(F^2)$ is used only for calculating R-factors(gt) etc. and is not relevant to the choice of reflections for refinement. R-factors based on F^2 are statistically about twice as large as those based on F, and R-factors based on ALL data will be even larger.

All esds (except the esd in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell esds are taken into account individually in the estimation of esds in distances, angles and torsion angles; correlations between esds in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell esds is used for estimating esds involving l.s. planes.

Figure 1. Fully-labeled displacement ellipsoid (50%) representation of $[PhB(CH_2PPh_2)_3]NiI \cdot (0.5)C_6H_6$ (**2 · (0.5)C_6H_6**) (hydrogens omitted for clarity).

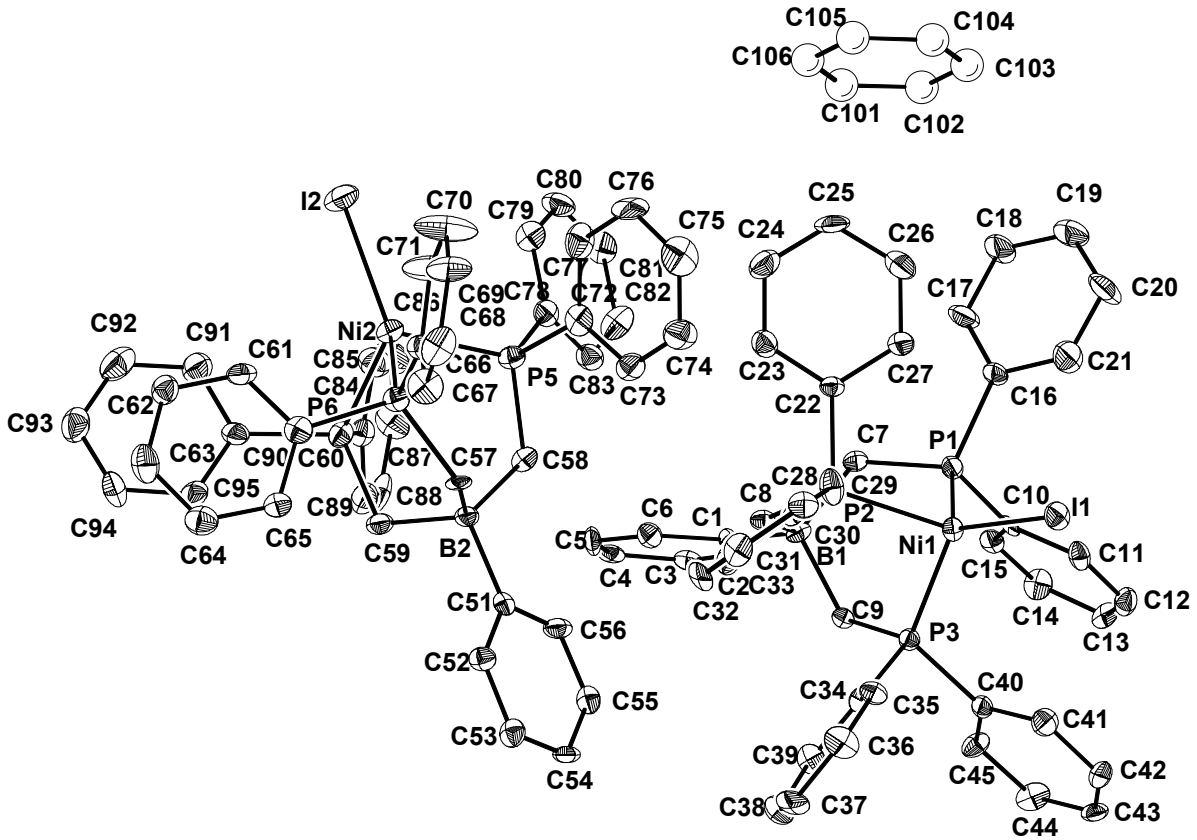


Table 1. Crystal data and structure refinement for $2 \cdot (0.5)C_6H_6$.

Empirical formula	$C_{48}H_{44}BINiP_3$	
Moiety formula	$C_{45}H_{41}BINiP_3$, $0.5C_6H_6$	
Formula weight	910.16	
Crystal habit	blade	
Crystal color	olive green	
Crystal size	0.22 x 0.16 x 0.15 mm^3	
Data Collection		
Type of diffractometer	CCD area detector	
Wavelength	0.71073 Å	
Temperature	98(2) K	
Unit cell dimensions	a = 22.502(3) Å	α = 90°
	b = 12.694(2) Å	β = 90.418(12)°
	c = 29.393(7) Å	γ = 90°
Volume	8396(3) $Å^3$	
Z	8	
Crystal system	Monoclinic	
Space group	$P2_1/c$	
Density (calculated)	1.440 g/cm^3	
F(000)	3704	
θ range for data collection	1.65 to 28.81°	
Completeness to θ = 28.81°	60.5%	
Index ranges	$-26 \le h \le 28$, $-13 \le k \le 15$, $-39 \le l \le 4$	
Reflections collected	19087	
Independent reflections	13261 [R(int) = 0.0619]	
Absorption coefficient	1.345 mm^{-1}	
Absorption correction	None	
Structure solution and refinement		
Structure solution program	SHELXS-97 (Sheldrick, 1990)	
Primary solution method	direct methods	
Secondary solution method	difference Fourier map	
Hydrogen placement	calculated postions	
Structure refinement program	SHELXL-97 (Sheldrick, 1997)	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	13261 / 0 / 931	
Goodness-of-fit on F^2	1.107	
Final R indices [$I>2\sigma(I)$]	R1 = 0.0494, wR2 = 0.0824	
R indices (all data)	R1 = 0.1013, wR2 = 0.0914	
Type of weighting scheme used	calculated	
Weighting scheme used	$w=1/[\sigma^2(F_o^2)]$	
Max shift/error	11.250	
Average shift/error	0.016	
Largest diff. peak and hole	0.891 and -0.871 $e \cdot Å^{-3}$	

Additional Refinement Details: The structure contains a solvent molecule which appears to be benzene. Attempts to refine the solvent anisotropically or with partial occupancy result in an unstable refinement. Consequently, the solvent molecule was refined isotropically.

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$ x 10^3) for 2 · (0.5)C_6H_6. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
Ni(1)	8684(1)	2672(1)	3147(1)	16(1)
I(1)	8602(1)	3032(1)	2314(1)	23(1)
P(1)	8369(1)	1153(2)	3488(1)	16(1)
P(2)	8180(1)	3728(2)	3632(1)	17(1)
P(3)	9519(1)	2704(2)	3582(1)	14(1)
B(1)	8662(3)	2284(7)	4321(2)	16(2)
C(1)	8698(3)	2059(6)	4877(2)	16(2)
C(2)	8917(3)	1129(5)	5043(2)	16(2)
C(3)	8968(3)	902(6)	5497(2)	23(2)
C(4)	8783(3)	1656(6)	5815(2)	20(2)
C(5)	8570(3)	2588(6)	5667(2)	22(2)
C(6)	8532(3)	2819(6)	5204(2)	20(2)
C(7)	8237(3)	1375(5)	4086(2)	19(2)
C(8)	8407(3)	3494(5)	4218(2)	16(2)
C(9)	9367(3)	2206(5)	4147(2)	15(2)
C(10)	8966(3)	218(5)	3425(2)	14(2)
C(11)	9251(3)	136(5)	3008(2)	19(2)
C(12)	9718(3)	-570(6)	2943(2)	24(2)
C(13)	9887(3)	-1215(6)	3280(2)	19(2)
C(14)	9599(3)	-1193(6)	3694(2)	23(2)
C(15)	9157(3)	-504(6)	3766(2)	18(2)
C(16)	7737(3)	438(6)	3265(2)	20(2)
C(17)	7324(3)	-62(6)	3545(2)	30(2)
C(18)	6883(3)	-672(6)	3375(2)	38(2)
C(19)	6820(3)	-811(7)	2903(2)	39(2)
C(20)	7225(4)	-356(7)	2620(2)	40(2)
C(21)	7666(3)	270(6)	2791(2)	35(2)
C(22)	7403(3)	3442(5)	3580(2)	16(2)
C(23)	6995(3)	3716(6)	3914(2)	23(2)
C(24)	6396(3)	3499(6)	3871(2)	32(2)
C(25)	6175(3)	3008(7)	3487(2)	35(2)
C(26)	6569(3)	2740(7)	3145(2)	42(3)
C(27)	7164(3)	2937(6)	3189(2)	33(2)
C(28)	8192(3)	5160(5)	3538(2)	14(2)
C(29)	7956(3)	5556(6)	3133(2)	26(2)
C(30)	7961(3)	6630(6)	3057(2)	22(2)
C(31)	8197(3)	7327(6)	3372(2)	24(2)
C(32)	8427(3)	6931(6)	3774(2)	22(2)
C(33)	8432(3)	5843(6)	3857(2)	24(2)
C(34)	9814(3)	4018(5)	3639(2)	16(2)
C(35)	9684(3)	4796(6)	3323(2)	20(2)
C(36)	9944(3)	5766(6)	3341(2)	30(2)
C(37)	10360(3)	6010(6)	3687(2)	27(2)
C(38)	10496(3)	5234(6)	4005(2)	25(2)
C(39)	10224(3)	4265(6)	3985(2)	23(2)
C(40)	10167(3)	2023(6)	3355(2)	18(2)
C(41)	10310(3)	2168(6)	2904(2)	24(2)
C(42)	10808(3)	1697(6)	2719(2)	24(2)
C(43)	11168(3)	1070(6)	2980(2)	20(2)
C(44)	11027(3)	913(5)	3428(2)	23(2)
C(45)	10533(3)	1400(6)	3621(2)	20(2)
Ni(2)	6301(1)	7030(1)	5568(1)	20(1)
I(2)	5257(1)	6761(1)	5803(1)	33(1)

P(4)	6678(1)	8465(2)	5218(1)	20(1)
P(5)	6706(1)	5899(2)	5075(1)	19(1)
P(6)	7088(1)	6976(2)	6056(1)	21(1)
B(2)	7781(4)	7246(7)	5223(2)	20(2)
C(51)	8485(3)	7270(6)	5073(2)	14(2)
C(52)	8801(3)	8199(6)	5038(2)	20(2)
C(53)	9396(3)	8237(6)	4918(2)	22(2)
C(54)	9699(3)	7323(6)	4825(2)	20(2)
C(55)	9390(3)	6385(6)	4860(2)	20(2)
C(56)	8812(3)	6356(6)	4987(2)	22(2)
C(57)	7405(3)	8201(5)	4972(2)	16(2)
C(58)	7499(3)	6046(5)	5081(2)	18(2)
C(59)	7766(3)	7426(6)	5782(2)	20(2)
C(60)	6746(3)	9492(6)	5650(2)	23(2)
C(61)	6259(3)	9629(6)	5932(2)	25(2)
C(62)	6250(3)	10389(6)	6270(2)	25(2)
C(63)	6749(4)	11011(6)	6332(2)	33(2)
C(64)	7245(3)	10890(6)	6052(2)	29(2)
C(65)	7251(3)	10150(6)	5712(2)	25(2)
C(66)	6210(3)	9129(6)	4798(2)	22(2)
C(67)	6420(4)	10035(6)	4570(2)	32(2)
C(68)	6052(4)	10586(6)	4275(2)	35(2)
C(69)	5489(4)	10260(7)	4193(2)	39(2)
C(70)	5266(4)	9372(8)	4405(3)	59(3)
C(71)	5629(4)	8835(7)	4713(3)	48(3)
C(72)	6428(3)	6139(6)	4498(2)	23(2)
C(73)	6796(3)	6398(5)	4132(2)	25(2)
C(74)	6553(4)	6570(6)	3701(2)	33(2)
C(75)	5951(4)	6471(7)	3629(2)	40(2)
C(76)	5577(3)	6200(7)	3983(2)	37(2)
C(77)	5820(4)	6047(6)	4415(2)	33(2)
C(78)	6535(3)	4513(6)	5161(2)	21(2)
C(79)	5960(3)	4161(6)	5265(2)	23(2)
C(80)	5847(3)	3116(6)	5319(2)	29(2)
C(81)	6292(3)	2371(6)	5284(2)	27(2)
C(82)	6858(3)	2682(6)	5188(2)	29(2)
C(83)	6991(3)	3755(6)	5127(2)	23(2)
C(84)	7233(3)	5665(6)	6268(2)	20(2)
C(85)	6767(4)	4951(6)	6287(2)	31(2)
C(86)	6860(4)	3895(7)	6455(2)	34(2)
C(87)	7402(4)	3610(6)	6611(2)	31(2)
C(88)	7871(4)	4324(7)	6594(2)	32(2)
C(89)	7789(4)	5348(6)	6426(2)	28(2)
C(90)	6934(3)	7733(6)	6573(2)	21(2)
C(91)	6420(3)	7513(6)	6811(2)	30(2)
C(92)	6273(4)	8109(7)	7190(2)	39(2)
C(93)	6632(3)	8949(7)	7326(2)	36(2)
C(94)	7139(3)	9161(6)	7085(2)	32(2)
C(95)	7294(3)	8545(6)	6713(2)	26(2)
C(101)	4912(10)	4610(20)	2798(6)	382(16)
C(102)	5046(7)	4005(14)	2419(9)	630(30)
C(103)	4861(9)	4329(18)	1989(7)	321(13)
C(104)	4542(11)	5260(20)	1938(7)	2000(180)
C(105)	4407(9)	5865(16)	2318(12)	670(30)
C(106)	4592(9)	5540(20)	2748(9)	660(30)

Table 3. Selected bond lengths [Å] and angles [°] for 2 · (0.5)C_6H_6.

Ni(1)-P(1)	2.289(2)	P(2)-Ni(1)-P(3)	92.99(7)
Ni(1)-P(2)	2.2646(19)	P(2)-Ni(1)-P(1)	93.76(7)
Ni(1)-P(3)	2.2666(19)	P(3)-Ni(1)-P(1)	91.52(7)
Ni(1)-I(1)	2.4974(9)	P(2)-Ni(1)-I(1)	118.35(6)
Ni(1)-B(1)	3.484(6)	P(3)-Ni(1)-I(1)	127.20(5)
Ni(2)-P(5)	2.239(2)	P(1)-Ni(1)-I(1)	124.24(5)
Ni(2)-P(4)	2.261(2)	P(5)-Ni(2)-P(4)	93.77(7)
Ni(2)-P(6)	2.269(2)	P(5)-Ni(2)-P(6)	94.00(7)
Ni(2)-I(2)	2.4774(10)	P(4)-Ni(2)-P(6)	91.07(8)
Ni(2)-B(2)	3.499(8)	P(5)-Ni(2)-I(2)	118.91(6)
		P(4)-Ni(2)-I(2)	126.66(6)
		P(6)-Ni(2)-I(2)	123.88(5)

Table 4. Bond lengths [Å] and angles [°] for 2 · (0.5)C_6H_6.

Ni(1)-P(2)	2.2646(19)	C(21)-H(21)	0.9500
Ni(1)-P(3)	2.2666(19)	C(22)-C(23)	1.392(8)
Ni(1)-P(1)	2.289(2)	C(22)-C(27)	1.419(8)
Ni(1)-I(1)	2.4974(9)	C(23)-C(24)	1.381(9)
Ni(1)-B(1)	3.484(6)	C(23)-H(23)	0.9500
P(1)-C(10)	1.804(7)	C(24)-C(25)	1.377(9)
P(1)-C(7)	1.805(5)	C(24)-H(24)	0.9500
P(1)-C(16)	1.806(7)	C(25)-C(26)	1.388(9)
P(2)-C(22)	1.791(7)	C(25)-H(25)	0.9500
P(2)-C(8)	1.818(5)	C(26)-C(27)	1.367(9)
P(2)-C(28)	1.839(7)	C(26)-H(26)	0.9500
P(3)-C(34)	1.802(7)	C(27)-H(27)	0.9500
P(3)-C(9)	1.811(5)	C(28)-C(33)	1.382(9)
P(3)-C(40)	1.825(7)	C(28)-C(29)	1.394(8)
B(1)-C(7)	1.647(10)	C(29)-C(30)	1.380(9)
B(1)-C(1)	1.662(8)	C(29)-H(29)	0.9500
B(1)-C(8)	1.667(10)	C(30)-C(31)	1.384(9)
B(1)-C(9)	1.673(9)	C(30)-H(30)	0.9500
C(1)-C(2)	1.368(8)	C(31)-C(32)	1.381(8)
C(1)-C(6)	1.415(8)	C(31)-H(31)	0.9500
C(2)-C(3)	1.369(7)	C(32)-C(33)	1.403(9)
C(2)-H(2)	0.9500	C(32)-H(32)	0.9500
C(3)-C(4)	1.403(9)	C(33)-H(33)	0.9500
C(3)-H(3)	0.9500	C(34)-C(35)	1.385(8)
C(4)-C(5)	1.348(9)	C(34)-C(39)	1.405(8)
C(4)-H(4)	0.9500	C(35)-C(36)	1.364(9)
C(5)-C(6)	1.394(7)	C(35)-H(35)	0.9500
C(5)-H(5)	0.9500	C(36)-C(37)	1.410(9)
C(6)-H(6)	0.9500	C(36)-H(36)	0.9500
C(7)-H(7A)	0.9900	C(37)-C(38)	1.392(9)
C(7)-H(7B)	0.9900	C(37)-H(37)	0.9500
C(8)-H(8A)	0.9900	C(38)-C(39)	1.375(9)
C(8)-H(8B)	0.9900	C(38)-H(38)	0.9500
C(9)-H(9A)	0.9900	C(39)-H(39)	0.9500
C(9)-H(9B)	0.9900	C(40)-C(41)	1.377(7)
C(10)-C(11)	1.392(7)	C(40)-C(45)	1.380(8)
C(10)-C(15)	1.421(8)	C(41)-C(42)	1.386(8)
C(11)-C(12)	1.395(9)	C(41)-H(41)	0.9500
C(11)-H(11)	0.9500	C(42)-C(43)	1.366(9)
C(12)-C(13)	1.338(9)	C(42)-H(42)	0.9500
C(12)-H(12)	0.9500	C(43)-C(44)	1.371(7)
C(13)-C(14)	1.382(8)	C(43)-H(43)	0.9500
C(13)-H(13)	0.9500	C(44)-C(45)	1.397(8)
C(14)-C(15)	1.344(9)	C(44)-H(44)	0.9500
C(14)-H(14)	0.9500	C(45)-H(45)	0.9500
C(15)-H(15)	0.9500	Ni(2)-P(5)	2.239(2)
C(16)-C(17)	1.397(8)	Ni(2)-P(4)	2.261(2)
C(16)-C(21)	1.416(8)	Ni(2)-P(6)	2.269(2)
C(17)-C(18)	1.352(9)	Ni(2)-I(2)	2.4774(10)
C(17)-H(17)	0.9500	Ni(2)-B(2)	3.499(8)
C(18)-C(19)	1.403(8)	P(4)-C(66)	1.824(7)
C(18)-H(18)	0.9500	P(4)-C(60)	1.825(7)
C(19)-C(20)	1.367(9)	P(4)-C(57)	1.825(6)
C(19)-H(19)	0.9500	P(5)-C(58)	1.794(7)
C(20)-C(21)	1.366(9)	P(5)-C(78)	1.819(7)
C(20)-H(20)	0.9500	P(5)-C(72)	1.830(7)

P(6)-C(84)	1.806(7)	C(78)-C(83)	1.411(9)
P(6)-C(59)	1.823(6)	C(79)-C(80)	1.360(9)
P(6)-C(90)	1.834(6)	C(79)-H(79)	0.9500
B(2)-C(57)	1.648(10)	C(80)-C(81)	1.382(9)
B(2)-C(51)	1.648(10)	C(80)-H(80)	0.9500
B(2)-C(59)	1.660(8)	C(81)-C(82)	1.365(9)
B(2)-C(58)	1.701(10)	C(81)-H(81)	0.9500
C(51)-C(52)	1.381(9)	C(82)-C(83)	1.406(9)
C(51)-C(56)	1.398(9)	C(82)-H(82)	0.9500
C(52)-C(53)	1.390(9)	C(83)-H(83)	0.9500
C(52)-H(52)	0.9500	C(84)-C(85)	1.386(9)
C(53)-C(54)	1.374(9)	C(84)-C(89)	1.393(9)
C(53)-H(53)	0.9500	C(85)-C(86)	1.443(10)
C(54)-C(55)	1.384(9)	C(85)-H(85)	0.9500
C(54)-H(54)	0.9500	C(86)-C(87)	1.349(9)
C(55)-C(56)	1.355(8)	C(86)-H(86)	0.9500
C(55)-H(55)	0.9500	C(87)-C(88)	1.392(10)
C(56)-H(56)	0.9500	C(87)-H(87)	0.9500
C(57)-H(57A)	0.9900	C(88)-C(89)	1.401(9)
C(57)-H(57B)	0.9900	C(88)-H(88)	0.9500
C(58)-H(58A)	0.9900	C(89)-H(89)	0.9500
C(58)-H(58B)	0.9900	C(90)-C(95)	1.374(9)
C(59)-H(59A)	0.9900	C(90)-C(91)	1.384(9)
C(59)-H(59B)	0.9900	C(91)-C(92)	1.388(9)
C(60)-C(61)	1.392(9)	C(91)-H(91)	0.9500
C(60)-C(65)	1.421(9)	C(92)-C(93)	1.396(10)
C(61)-C(62)	1.386(9)	C(92)-H(92)	0.9500
C(61)-H(61)	0.9500	C(93)-C(94)	1.375(10)
C(62)-C(63)	1.383(9)	C(93)-H(93)	0.9500
C(62)-H(62)	0.9500	C(94)-C(95)	1.391(8)
C(63)-C(64)	1.399(9)	C(94)-H(94)	0.9500
C(63)-H(63)	0.9500	C(95)-H(95)	0.9500
C(64)-C(65)	1.372(9)	C(101)-C(102)	1.3900
C(64)-H(64)	0.9500	C(101)-C(106)	1.3900
C(65)-H(65)	0.9500	C(101)-H(101)	0.9500
C(66)-C(71)	1.380(9)	C(102)-C(103)	1.3900
C(66)-C(67)	1.412(10)	C(102)-H(102)	0.9500
C(67)-C(68)	1.385(9)	C(103)-C(104)	1.3900
C(67)-H(67)	0.9500	C(103)-H(103)	0.9500
C(68)-C(69)	1.352(9)	C(104)-C(105)	1.3900
C(68)-H(68)	0.9500	C(104)-H(104)	0.9500
C(69)-C(70)	1.385(11)	C(105)-C(106)	1.3900
C(69)-H(69)	0.9500	C(105)-H(105)	0.9500
C(70)-C(71)	1.392(10)	C(106)-H(106)	0.9500
C(70)-H(70)	0.9500		
C(71)-H(71)	0.9500	P(2)-Ni(1)-P(3)	92.99(7)
C(72)-C(77)	1.393(10)	P(2)-Ni(1)-P(1)	93.76(7)
C(72)-C(73)	1.402(8)	P(3)-Ni(1)-P(1)	91.52(7)
C(73)-C(74)	1.395(8)	P(2)-Ni(1)-I(1)	118.35(6)
C(73)-H(73)	0.9500	P(3)-Ni(1)-I(1)	127.20(5)
C(74)-C(75)	1.375(10)	P(1)-Ni(1)-I(1)	124.24(5)
C(74)-H(74)	0.9500	P(2)-Ni(1)-B(1)	56.71(14)
C(75)-C(76)	1.386(9)	P(3)-Ni(1)-B(1)	57.46(13)
C(75)-H(75)	0.9500	P(1)-Ni(1)-B(1)	55.99(14)
C(76)-C(77)	1.394(8)	I(1)-Ni(1)-B(1)	174.43(13)
C(76)-H(76)	0.9500	C(10)-P(1)-C(7)	109.4(3)
C(77)-H(77)	0.9500	C(10)-P(1)-C(16)	102.6(3)
C(78)-C(79)	1.403(9)	C(7)-P(1)-C(16)	107.3(3)

C(10)-P(1)-Ni(1)	106.0(2)	B(1)-C(9)-H(9B)	108.2
C(7)-P(1)-Ni(1)	110.3(2)	P(3)-C(9)-H(9B)	108.2
C(16)-P(1)-Ni(1)	120.6(2)	H(9A)-C(9)-H(9B)	107.3
C(22)-P(2)-C(8)	108.3(3)	C(11)-C(10)-C(15)	115.7(6)
C(22)-P(2)-C(28)	101.7(3)	C(11)-C(10)-P(1)	119.3(5)
C(8)-P(2)-C(28)	107.3(3)	C(15)-C(10)-P(1)	124.9(5)
C(22)-P(2)-Ni(1)	108.7(2)	C(10)-C(11)-C(12)	121.3(6)
C(8)-P(2)-Ni(1)	111.1(2)	C(10)-C(11)-H(11)	119.3
C(28)-P(2)-Ni(1)	118.9(2)	C(12)-C(11)-H(11)	119.3
C(34)-P(3)-C(9)	108.1(3)	C(13)-C(12)-C(11)	120.2(6)
C(34)-P(3)-C(40)	100.2(3)	C(13)-C(12)-H(12)	119.9
C(9)-P(3)-C(40)	109.1(3)	C(11)-C(12)-H(12)	119.9
C(34)-P(3)-Ni(1)	111.8(2)	C(12)-C(13)-C(14)	120.5(7)
C(9)-P(3)-Ni(1)	110.4(2)	C(12)-C(13)-H(13)	119.8
C(40)-P(3)-Ni(1)	116.5(2)	C(14)-C(13)-H(13)	119.8
C(7)-B(1)-C(1)	108.5(5)	C(15)-C(14)-C(13)	120.2(6)
C(7)-B(1)-C(8)	111.8(5)	C(15)-C(14)-H(14)	119.9
C(1)-B(1)-C(8)	110.6(5)	C(13)-C(14)-H(14)	119.9
C(7)-B(1)-C(9)	112.3(5)	C(14)-C(15)-C(10)	122.0(6)
C(1)-B(1)-C(9)	104.5(5)	C(14)-C(15)-H(15)	119.0
C(8)-B(1)-C(9)	108.9(6)	C(10)-C(15)-H(15)	119.0
C(7)-B(1)-Ni(1)	72.3(3)	C(17)-C(16)-C(21)	116.1(7)
C(1)-B(1)-Ni(1)	176.0(5)	C(17)-C(16)-P(1)	122.6(5)
C(8)-B(1)-Ni(1)	72.4(3)	C(21)-C(16)-P(1)	121.0(5)
C(9)-B(1)-Ni(1)	71.7(3)	C(18)-C(17)-C(16)	122.2(6)
C(2)-C(1)-C(6)	116.3(5)	C(18)-C(17)-H(17)	118.9
C(2)-C(1)-B(1)	120.9(5)	C(16)-C(17)-H(17)	118.9
C(6)-C(1)-B(1)	122.7(6)	C(17)-C(18)-C(19)	120.4(7)
C(1)-C(2)-C(3)	123.8(6)	C(17)-C(18)-H(18)	119.8
C(1)-C(2)-H(2)	118.1	C(19)-C(18)-H(18)	119.8
C(3)-C(2)-H(2)	118.1	C(20)-C(19)-C(18)	119.1(8)
C(2)-C(3)-C(4)	118.9(7)	C(20)-C(19)-H(19)	120.5
C(2)-C(3)-H(3)	120.5	C(18)-C(19)-H(19)	120.5
C(4)-C(3)-H(3)	120.5	C(21)-C(20)-C(19)	120.4(7)
C(5)-C(4)-C(3)	119.3(6)	C(21)-C(20)-H(20)	119.8
C(5)-C(4)-H(4)	120.3	C(19)-C(20)-H(20)	119.8
C(3)-C(4)-H(4)	120.3	C(20)-C(21)-C(16)	121.8(7)
C(4)-C(5)-C(6)	121.2(6)	C(20)-C(21)-H(21)	119.1
C(4)-C(5)-H(5)	119.4	C(16)-C(21)-H(21)	119.1
C(6)-C(5)-H(5)	119.4	C(23)-C(22)-C(27)	115.8(7)
C(5)-C(6)-C(1)	120.4(7)	C(23)-C(22)-P(2)	122.6(5)
C(5)-C(6)-H(6)	119.8	C(27)-C(22)-P(2)	121.6(5)
C(1)-C(6)-H(6)	119.8	C(24)-C(23)-C(22)	122.3(6)
B(1)-C(7)-P(1)	114.8(4)	C(24)-C(23)-H(23)	118.9
B(1)-C(7)-H(7A)	108.6	C(22)-C(23)-H(23)	118.9
P(1)-C(7)-H(7A)	108.6	C(25)-C(24)-C(23)	120.7(7)
B(1)-C(7)-H(7B)	108.6	C(25)-C(24)-H(24)	119.6
P(1)-C(7)-H(7B)	108.6	C(23)-C(24)-H(24)	119.6
H(7A)-C(7)-H(7B)	107.6	C(24)-C(25)-C(26)	118.4(7)
B(1)-C(8)-P(2)	114.6(4)	C(24)-C(25)-H(25)	120.8
B(1)-C(8)-H(8A)	108.6	C(26)-C(25)-H(25)	120.8
P(2)-C(8)-H(8A)	108.6	C(27)-C(26)-C(25)	121.1(7)
B(1)-C(8)-H(8B)	108.6	C(27)-C(26)-H(26)	119.5
P(2)-C(8)-H(8B)	108.6	C(25)-C(26)-H(26)	119.5
H(8A)-C(8)-H(8B)	107.6	C(26)-C(27)-C(22)	121.7(6)
B(1)-C(9)-P(3)	116.5(4)	C(26)-C(27)-H(27)	119.2
B(1)-C(9)-H(9A)	108.2	C(22)-C(27)-H(27)	119.2
P(3)-C(9)-H(9A)	108.2	C(33)-C(28)-C(29)	119.7(6)

C(33)-C(28)-P(2)	121.7(5)	P(6)-Ni(2)-I(2)	123.88(5)
C(29)-C(28)-P(2)	118.6(5)	P(5)-Ni(2)-B(2)	57.95(14)
C(30)-C(29)-C(28)	119.4(6)	P(4)-Ni(2)-B(2)	56.21(15)
C(30)-C(29)-H(29)	120.3	P(6)-Ni(2)-B(2)	56.37(12)
C(28)-C(29)-H(29)	120.3	I(2)-Ni(2)-B(2)	176.53(15)
C(29)-C(30)-C(31)	121.8(6)	C(66)-P(4)-C(60)	100.7(3)
C(29)-C(30)-H(30)	119.1	C(66)-P(4)-C(57)	109.4(3)
C(31)-C(30)-H(30)	119.1	C(60)-P(4)-C(57)	109.6(3)
C(32)-C(31)-C(30)	118.6(7)	C(66)-P(4)-Ni(2)	117.7(3)
C(32)-C(31)-H(31)	120.7	C(60)-P(4)-Ni(2)	106.8(2)
C(30)-C(31)-H(31)	120.7	C(57)-P(4)-Ni(2)	111.9(2)
C(31)-C(32)-C(33)	120.6(6)	C(58)-P(5)-C(78)	108.1(3)
C(31)-C(32)-H(32)	119.7	C(58)-P(5)-C(72)	109.0(3)
C(33)-C(32)-H(32)	119.7	C(78)-P(5)-C(72)	102.6(3)
C(28)-C(33)-C(32)	119.8(6)	C(58)-P(5)-Ni(2)	109.7(2)
C(28)-C(33)-H(33)	120.1	C(78)-P(5)-Ni(2)	116.2(2)
C(32)-C(33)-H(33)	120.1	C(72)-P(5)-Ni(2)	110.9(2)
C(35)-C(34)-C(39)	117.4(7)	C(84)-P(6)-C(59)	106.9(3)
C(35)-C(34)-P(3)	121.5(5)	C(84)-P(6)-C(90)	103.4(3)
C(39)-C(34)-P(3)	120.9(5)	C(59)-P(6)-C(90)	111.4(3)
C(36)-C(35)-C(34)	122.0(6)	C(84)-P(6)-Ni(2)	112.6(3)
C(36)-C(35)-H(35)	119.0	C(59)-P(6)-Ni(2)	111.4(2)
C(34)-C(35)-H(35)	119.0	C(90)-P(6)-Ni(2)	110.9(2)
C(35)-C(36)-C(37)	120.5(7)	C(57)-B(2)-C(51)	110.9(5)
C(35)-C(36)-H(36)	119.7	C(57)-B(2)-C(59)	109.1(6)
C(37)-C(36)-H(36)	119.7	C(51)-B(2)-C(59)	106.8(5)
C(38)-C(37)-C(36)	118.0(7)	C(57)-B(2)-C(58)	111.1(5)
C(38)-C(37)-H(37)	121.0	C(51)-B(2)-C(58)	108.0(6)
C(36)-C(37)-H(37)	121.0	C(59)-B(2)-C(58)	110.9(5)
C(39)-C(38)-C(37)	120.6(7)	C(57)-B(2)-Ni(2)	72.6(3)
C(39)-C(38)-H(38)	119.7	C(51)-B(2)-Ni(2)	176.3(5)
C(37)-C(38)-H(38)	119.7	C(59)-B(2)-Ni(2)	72.4(3)
C(38)-C(39)-C(34)	121.4(6)	C(58)-B(2)-Ni(2)	69.4(3)
C(38)-C(39)-H(39)	119.3	C(52)-C(51)-C(56)	115.1(6)
C(34)-C(39)-H(39)	119.3	C(52)-C(51)-B(2)	122.1(6)
C(41)-C(40)-C(45)	118.6(6)	C(56)-C(51)-B(2)	122.7(6)
C(41)-C(40)-P(3)	118.8(5)	C(51)-C(52)-C(53)	123.1(7)
C(45)-C(40)-P(3)	122.5(4)	C(51)-C(52)-H(52)	118.5
C(40)-C(41)-C(42)	121.0(6)	C(53)-C(52)-H(52)	118.5
C(40)-C(41)-H(41)	119.5	C(54)-C(53)-C(52)	120.1(7)
C(42)-C(41)-H(41)	119.5	C(54)-C(53)-H(53)	119.9
C(43)-C(42)-C(41)	120.5(6)	C(52)-C(53)-H(53)	119.9
C(43)-C(42)-H(42)	119.7	C(53)-C(54)-C(55)	117.5(6)
C(41)-C(42)-H(42)	119.7	C(53)-C(54)-H(54)	121.3
C(42)-C(43)-C(44)	118.9(6)	C(55)-C(54)-H(54)	121.3
C(42)-C(43)-H(43)	120.5	C(56)-C(55)-C(54)	121.9(7)
C(44)-C(43)-H(43)	120.5	C(56)-C(55)-H(55)	119.1
C(43)-C(44)-C(45)	121.1(6)	C(54)-C(55)-H(55)	119.1
C(43)-C(44)-H(44)	119.5	C(55)-C(56)-C(51)	122.3(7)
C(45)-C(44)-H(44)	119.5	C(55)-C(56)-H(56)	118.8
C(40)-C(45)-C(44)	119.8(6)	C(51)-C(56)-H(56)	118.8
C(40)-C(45)-H(45)	120.1	B(2)-C(57)-P(4)	114.6(4)
C(44)-C(45)-H(45)	120.1	B(2)-C(57)-H(57A)	108.6
P(5)-Ni(2)-P(4)	93.77(7)	P(4)-C(57)-H(57A)	108.6
P(5)-Ni(2)-P(6)	94.00(7)	B(2)-C(57)-H(57B)	108.6
P(4)-Ni(2)-P(6)	91.07(8)	P(4)-C(57)-H(57B)	108.6
P(5)-Ni(2)-I(2)	118.91(6)	H(57A)-C(57)-H(57B)	107.6
P(4)-Ni(2)-I(2)	126.66(6)	B(2)-C(58)-P(5)	117.6(5)

B(2)-C(58)-H(58A)	107.9	C(76)-C(75)-H(75)	119.6
P(5)-C(58)-H(58A)	107.9	C(75)-C(76)-C(77)	118.9(8)
B(2)-C(58)-H(58B)	107.9	C(75)-C(76)-H(76)	120.6
P(5)-C(58)-H(58B)	107.9	C(77)-C(76)-H(76)	120.6
H(58A)-C(58)-H(58B)	107.2	C(72)-C(77)-C(76)	121.7(7)
B(2)-C(59)-P(6)	114.6(4)	C(72)-C(77)-H(77)	119.2
B(2)-C(59)-H(59A)	108.6	C(76)-C(77)-H(77)	119.2
P(6)-C(59)-H(59A)	108.6	C(79)-C(78)-C(83)	118.0(7)
B(2)-C(59)-H(59B)	108.6	C(79)-C(78)-P(5)	122.3(6)
P(6)-C(59)-H(59B)	108.6	C(83)-C(78)-P(5)	119.7(5)
H(59A)-C(59)-H(59B)	107.6	C(80)-C(79)-C(78)	120.6(7)
C(61)-C(60)-C(65)	118.9(6)	C(80)-C(79)-H(79)	119.7
C(61)-C(60)-P(4)	116.1(6)	C(78)-C(79)-H(79)	119.7
C(65)-C(60)-P(4)	124.9(5)	C(79)-C(80)-C(81)	121.5(7)
C(62)-C(61)-C(60)	122.0(7)	C(79)-C(80)-H(80)	119.2
C(62)-C(61)-H(61)	119.0	C(81)-C(80)-H(80)	119.3
C(60)-C(61)-H(61)	119.0	C(82)-C(81)-C(80)	119.7(7)
C(63)-C(62)-C(61)	118.4(7)	C(82)-C(81)-H(81)	120.2
C(63)-C(62)-H(62)	120.8	C(80)-C(81)-H(81)	120.2
C(61)-C(62)-H(62)	120.8	C(81)-C(82)-C(83)	120.4(7)
C(62)-C(63)-C(64)	120.7(7)	C(81)-C(82)-H(82)	119.8
C(62)-C(63)-H(63)	119.7	C(83)-C(82)-H(82)	119.8
C(64)-C(63)-H(63)	119.7	C(82)-C(83)-C(78)	119.8(7)
C(65)-C(64)-C(63)	121.1(8)	C(82)-C(83)-H(83)	120.1
C(65)-C(64)-H(64)	119.5	C(78)-C(83)-H(83)	120.1
C(63)-C(64)-H(64)	119.5	C(85)-C(84)-C(89)	118.4(7)
C(64)-C(65)-C(60)	118.9(6)	C(85)-C(84)-P(6)	118.8(6)
C(64)-C(65)-H(65)	120.6	C(89)-C(84)-P(6)	122.8(6)
C(60)-C(65)-H(65)	120.6	C(84)-C(85)-C(86)	120.9(7)
C(71)-C(66)-C(67)	117.0(7)	C(84)-C(85)-H(85)	119.5
C(71)-C(66)-P(4)	122.5(6)	C(86)-C(85)-H(85)	119.5
C(67)-C(66)-P(4)	120.2(6)	C(87)-C(86)-C(85)	119.5(8)
C(68)-C(67)-C(66)	120.5(8)	C(87)-C(86)-H(86)	120.2
C(68)-C(67)-H(67)	119.8	C(85)-C(86)-H(86)	120.2
C(66)-C(67)-H(67)	119.8	C(86)-C(87)-C(88)	119.8(8)
C(69)-C(68)-C(67)	120.9(8)	C(86)-C(87)-H(87)	120.1
C(69)-C(68)-H(68)	119.6	C(88)-C(87)-H(87)	120.1
C(67)-C(68)-H(68)	119.6	C(87)-C(88)-C(89)	121.3(8)
C(68)-C(69)-C(70)	120.6(8)	C(87)-C(88)-H(88)	119.4
C(68)-C(69)-H(69)	119.7	C(89)-C(88)-H(88)	119.4
C(70)-C(69)-H(69)	119.7	C(84)-C(89)-C(88)	120.0(8)
C(69)-C(70)-C(71)	118.7(8)	C(84)-C(89)-H(89)	120.0
C(69)-C(70)-H(70)	120.6	C(88)-C(89)-H(89)	120.0
C(71)-C(70)-H(70)	120.6	C(95)-C(90)-C(91)	119.5(6)
C(66)-C(71)-C(70)	122.3(8)	C(95)-C(90)-P(6)	121.9(5)
C(66)-C(71)-H(71)	118.9	C(91)-C(90)-P(6)	118.5(6)
C(70)-C(71)-H(71)	118.9	C(90)-C(91)-C(92)	120.1(7)
C(77)-C(72)-C(73)	118.2(6)	C(90)-C(91)-H(91)	119.9
C(77)-C(72)-P(5)	118.4(5)	C(92)-C(91)-H(91)	120.0
C(73)-C(72)-P(5)	123.4(6)	C(91)-C(92)-C(93)	120.4(7)
C(74)-C(73)-C(72)	120.2(8)	C(91)-C(92)-H(92)	119.8
C(74)-C(73)-H(73)	119.9	C(93)-C(92)-H(92)	119.8
C(72)-C(73)-H(73)	119.9	C(94)-C(93)-C(92)	118.8(7)
C(75)-C(74)-C(73)	120.3(7)	C(94)-C(93)-H(93)	120.6
C(75)-C(74)-H(74)	119.9	C(92)-C(93)-H(93)	120.6
C(73)-C(74)-H(74)	119.9	C(93)-C(94)-C(95)	120.6(8)
C(74)-C(75)-C(76)	120.7(6)	C(93)-C(94)-H(94)	119.7
C(74)-C(75)-H(75)	119.6	C(95)-C(94)-H(94)	119.7

C(90)-C(95)-C(94)	120.5(7)	C(104)-C(103)-H(103)	120.0
C(90)-C(95)-H(95)	119.7	C(105)-C(104)-C(103)	120.0
C(94)-C(95)-H(95)	119.7	C(105)-C(104)-H(104)	120.0
C(102)-C(101)-C(106)	120.0	C(103)-C(104)-H(104)	120.0
C(102)-C(101)-H(101)	119.8	C(104)-C(105)-C(106)	120.0
C(106)-C(101)-H(101)	120.2	C(104)-C(105)-H(105)	120.0
C(103)-C(102)-C(101)	120.0	C(106)-C(105)-H(105)	120.0
C(103)-C(102)-H(102)	120.0	C(105)-C(106)-C(101)	120.0
C(101)-C(102)-H(102)	120.0	C(105)-C(106)-H(106)	120.0
C(102)-C(103)-C(104)	120.0	C(101)-C(106)-H(106)	120.0
C(102)-C(103)-H(103)	120.0		

Table 5. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for $2 \cdot (0.5)C_6H_6$. The anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U^{11} + ... + 2\ h\ k\ a^*\ b^*\ U^{12}]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Ni(1)	19(1)	14(1)	14(1)	-1(1)	1(1)	-1(1)
I(1)	27(1)	26(1)	15(1)	2(1)	1(1)	-5(1)
P(1)	18(1)	17(1)	15(1)	-2(1)	0(1)	-3(1)
P(2)	18(1)	17(1)	16(1)	0(1)	1(1)	2(1)
P(3)	16(1)	13(1)	15(1)	-1(1)	1(1)	-2(1)
B(1)	11(5)	21(6)	16(3)	5(3)	2(3)	1(4)
C(1)	17(5)	14(5)	17(3)	-6(3)	3(3)	-4(4)
C(2)	21(5)	10(5)	17(3)	-1(3)	8(3)	-1(4)
C(3)	16(5)	25(5)	27(4)	-2(3)	-1(3)	-8(4)
C(4)	15(5)	29(5)	15(3)	5(3)	0(3)	-13(4)
C(5)	25(5)	29(5)	13(3)	-10(3)	-2(3)	4(4)
C(6)	20(5)	20(5)	17(3)	0(3)	-2(3)	0(4)
C(7)	15(5)	20(5)	20(3)	-1(3)	4(3)	-5(4)
C(8)	14(4)	16(5)	17(3)	3(3)	0(3)	-2(4)
C(9)	13(4)	18(5)	15(3)	-1(3)	-2(2)	0(4)
C(10)	18(5)	7(4)	18(3)	-7(3)	0(3)	-9(4)
C(11)	29(5)	12(5)	17(3)	-2(3)	1(3)	-3(4)
C(12)	28(5)	18(5)	25(4)	-7(3)	10(3)	-6(4)
C(13)	18(5)	6(5)	34(4)	-2(3)	7(3)	4(4)
C(14)	28(5)	18(5)	25(3)	4(3)	-1(3)	7(4)
C(15)	22(5)	17(5)	16(3)	1(3)	3(3)	-10(4)
C(16)	20(5)	17(5)	22(3)	-3(3)	1(3)	-9(4)
C(17)	24(5)	40(6)	25(4)	-3(3)	-4(3)	-17(5)
C(18)	38(6)	43(6)	32(4)	-9(4)	8(3)	-29(5)
C(19)	31(6)	43(7)	42(5)	-6(4)	0(4)	-19(5)
C(20)	44(6)	56(7)	21(4)	-5(4)	-7(3)	-29(5)
C(21)	38(6)	44(6)	22(4)	-2(3)	6(3)	-15(5)
C(22)	13(4)	18(5)	17(3)	2(3)	0(3)	-3(4)
C(23)	26(5)	21(5)	22(3)	-2(3)	0(3)	-4(4)
C(24)	26(6)	35(6)	35(4)	-3(3)	13(3)	-5(5)
C(25)	9(5)	61(7)	34(4)	-2(4)	-1(3)	-6(5)
C(26)	32(6)	65(7)	30(4)	-14(4)	-2(3)	-18(5)
C(27)	20(5)	57(7)	23(3)	-12(4)	4(3)	-10(5)
C(28)	15(5)	7(5)	22(3)	0(3)	4(3)	5(4)
C(29)	43(6)	16(5)	19(3)	-1(3)	1(3)	0(5)
C(30)	21(5)	22(5)	23(3)	5(3)	-4(3)	3(4)
C(31)	34(6)	7(5)	32(4)	3(3)	6(3)	3(4)
C(32)	33(5)	10(5)	24(3)	-5(3)	2(3)	-14(4)
C(33)	27(5)	28(5)	17(3)	1(3)	2(3)	7(5)
C(34)	19(5)	15(5)	14(3)	3(3)	3(3)	1(4)
C(35)	19(5)	17(5)	23(3)	1(3)	-2(3)	-5(4)
C(36)	36(6)	27(6)	28(4)	8(3)	-6(3)	-5(5)
C(37)	24(6)	15(5)	41(4)	-2(3)	0(3)	-12(4)
C(38)	28(5)	22(5)	25(4)	2(3)	-7(3)	-1(4)
C(39)	28(5)	13(5)	26(4)	2(3)	-1(3)	1(4)
C(40)	19(5)	16(5)	18(3)	-5(3)	4(3)	-6(4)
C(41)	23(5)	31(6)	18(3)	1(3)	-2(3)	3(4)
C(42)	22(5)	34(6)	15(3)	-2(3)	6(3)	-2(4)
C(43)	9(5)	18(5)	34(4)	-5(3)	2(3)	1(4)
C(44)	23(5)	11(5)	36(4)	10(3)	3(3)	3(4)
C(45)	15(5)	24(5)	21(3)	6(3)	2(3)	7(4)
Ni(2)	16(1)	21(1)	24(1)	2(1)	3(1)	1(1)
I(2)	20(1)	35(1)	42(1)	1(1)	9(1)	-1(1)

P(4)	20(1)	15(1)	25(1)	1(1)	1(1)	-1(1)
P(5)	16(1)	18(1)	23(1)	1(1)	0(1)	1(1)
P(6)	20(1)	23(1)	19(1)	1(1)	3(1)	1(1)
B(2)	14(5)	31(6)	14(3)	0(3)	1(3)	-5(5)
C(51)	15(4)	13(5)	13(3)	1(3)	-6(2)	5(4)
C(52)	19(5)	15(5)	25(3)	1(3)	1(3)	-1(4)
C(53)	24(5)	19(5)	24(3)	-2(3)	0(3)	5(4)
C(54)	10(4)	32(5)	17(3)	2(3)	-1(3)	-5(4)
C(55)	23(5)	18(5)	19(3)	-1(3)	-4(3)	7(4)
C(56)	14(5)	34(6)	18(3)	5(3)	0(3)	-7(4)
C(57)	8(4)	13(5)	26(3)	1(3)	4(3)	-6(4)
C(58)	18(5)	15(5)	21(3)	3(3)	4(3)	2(4)
C(59)	14(5)	23(5)	23(3)	1(3)	2(3)	-3(4)
C(60)	22(5)	19(5)	27(4)	1(3)	-2(3)	4(4)
C(61)	14(5)	29(6)	33(4)	-3(3)	1(3)	-3(4)
C(62)	27(5)	21(5)	28(4)	-3(3)	4(3)	1(4)
C(63)	51(6)	16(5)	32(4)	-4(3)	2(4)	0(5)
C(64)	26(5)	28(6)	34(4)	2(3)	-3(3)	2(5)
C(65)	20(5)	29(6)	25(4)	-2(3)	3(3)	-4(4)
C(66)	19(5)	16(5)	30(4)	-1(3)	0(3)	-1(4)
C(67)	38(6)	23(6)	35(4)	8(3)	-4(3)	7(5)
C(68)	44(6)	27(6)	33(4)	11(3)	9(4)	9(5)
C(69)	15(6)	43(7)	59(5)	12(4)	-13(4)	10(5)
C(70)	23(7)	60(8)	93(7)	41(6)	-34(5)	-3(6)
C(71)	20(6)	40(7)	83(6)	29(5)	-14(4)	-3(6)
C(72)	30(6)	6(5)	32(4)	0(3)	0(3)	6(4)
C(73)	24(5)	19(5)	32(4)	0(3)	6(3)	-3(4)
C(74)	31(6)	43(6)	26(4)	7(3)	2(3)	-10(5)
C(75)	48(7)	46(7)	25(4)	13(3)	-9(4)	7(5)
C(76)	10(5)	65(7)	36(4)	1(4)	-9(3)	7(5)
C(77)	42(6)	40(6)	18(3)	4(3)	2(3)	4(5)
C(78)	24(5)	22(5)	16(3)	2(3)	1(3)	-3(4)
C(79)	27(5)	11(5)	31(4)	3(3)	3(3)	3(4)
C(80)	22(5)	25(6)	40(4)	-3(4)	-4(3)	-8(5)
C(81)	37(6)	11(5)	33(4)	2(3)	5(3)	-6(5)
C(82)	28(6)	22(6)	36(4)	8(3)	4(3)	17(5)
C(83)	23(5)	19(5)	27(4)	-2(3)	-1(3)	-3(4)
C(84)	24(5)	18(5)	19(3)	2(3)	3(3)	0(4)
C(85)	27(6)	34(6)	32(4)	-1(3)	-6(3)	1(5)
C(86)	37(6)	25(6)	39(4)	3(3)	-6(4)	-2(5)
C(87)	35(6)	22(6)	36(4)	2(3)	-9(4)	-1(5)
C(88)	37(6)	43(6)	18(3)	-1(3)	3(3)	27(5)
C(89)	30(6)	27(6)	27(4)	-3(3)	8(3)	-1(5)
C(90)	15(5)	26(5)	22(3)	0(3)	-4(3)	0(4)
C(91)	29(5)	26(6)	35(4)	-4(3)	6(3)	-2(5)
C(92)	33(6)	51(7)	34(4)	7(4)	11(3)	4(6)
C(93)	32(6)	52(7)	24(4)	-6(4)	-3(3)	13(5)
C(94)	43(6)	29(6)	23(4)	-9(3)	-3(3)	-4(5)
C(95)	16(5)	39(6)	24(3)	-2(3)	-1(3)	8(4)

Table 6. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for 2 · (0.5)C_6H_6.

	x	y	z	U(eq)
H(2)	9040	610	4831	19
H(3)	9126	246	5595	27
H(4)	8808	1510	6132	24
H(5)	8443	3097	5883	27
H(6)	8394	3491	5108	23
H(7A)	7816	1582	4125	22
H(7B)	8298	704	4251	22
H(8A)	8721	4008	4300	19
H(8B)	8063	3627	4418	19
H(9A)	9490	1458	4158	18
H(9B)	9619	2597	4366	18
H(11)	9126	571	2762	23
H(12)	9916	-595	2659	28
H(13)	10207	-1691	3235	23
H(14)	9715	-1667	3929	28
H(15)	8965	-498	4053	22
H(17)	7355	29	3865	35
H(18)	6614	-1009	3576	45
H(19)	6500	-1215	2783	46
H(20)	7199	-476	2301	48
H(21)	7933	602	2587	42
H(23)	7134	4065	4180	28
H(24)	6133	3690	4108	39
H(25)	5763	2858	3458	42
H(26)	6423	2413	2876	51
H(27)	7423	2732	2952	40
H(29)	7794	5092	2912	31
H(30)	7798	6896	2781	27
H(31)	8201	8063	3313	29
H(32)	8583	7400	3996	27
H(33)	8600	5575	4131	29
H(35)	9406	4650	3087	24
H(36)	9844	6282	3119	36
H(37)	10542	6685	3701	32
H(38)	10779	5375	4239	30
H(39)	10315	3752	4210	27
H(41)	10063	2596	2717	28
H(42)	10901	1811	2408	29
H(43)	11510	748	2853	24
H(44)	11270	466	3610	28
H(45)	10448	1303	3934	24
H(52)	8601	8843	5099	24
H(53)	9595	8896	4900	27
H(54)	10105	7335	4739	24
H(55)	9588	5743	4794	24
H(56)	8622	5692	5018	27
H(57A)	7350	8018	4647	19
H(57B)	7645	8854	4986	19
H(58A)	7665	5521	5296	22
H(58B)	7647	5862	4774	22
H(59A)	7818	8186	5846	24
H(59B)	8108	7050	5920	24
H(61)	5921	9188	5891	31

H(62)	5910	10481	6456	30
H(63)	6755	11525	6567	40
H(64)	7583	11327	6098	35
H(65)	7588	10079	5521	29
H(67)	6816	10267	4620	38
H(68)	6196	11201	4129	42
H(69)	5244	10645	3987	47
H(70)	4874	9134	4343	71
H(71)	5471	8245	4871	57
H(73)	7213	6457	4178	30
H(74)	6804	6756	3455	40
H(75)	5789	6589	3334	48
H(76)	5162	6120	3931	45
H(77)	5564	5875	4660	40
H(79)	5648	4658	5299	28
H(80)	5453	2894	5382	35
H(81)	6204	1646	5326	32
H(82)	7164	2171	5163	34
H(83)	7386	3968	5063	27
H(85)	6382	5161	6189	37
H(86)	6542	3404	6455	41
H(87)	7463	2925	6731	37
H(88)	8253	4113	6699	39
H(89)	8114	5826	6421	34
H(91)	6168	6953	6715	36
H(92)	5925	7943	7357	47
H(93)	6528	9366	7582	43
H(94)	7386	9734	7173	38
H(95)	7652	8688	6555	32
H(101)	5038	4389	3092	459
H(102)	5265	3369	2453	758
H(103)	4953	3915	1729	385
H(104)	4415	5481	1644	2400
H(105)	4189	6501	2283	803
H(106)	4500	5955	3007	794

Figure 2. Fully-labeled displacement ellipsoid (50%) representation of [PhB($CH_2P^iPr_2$)$_3$]NiCl (**3**) (hydrogens omitted for clarity).

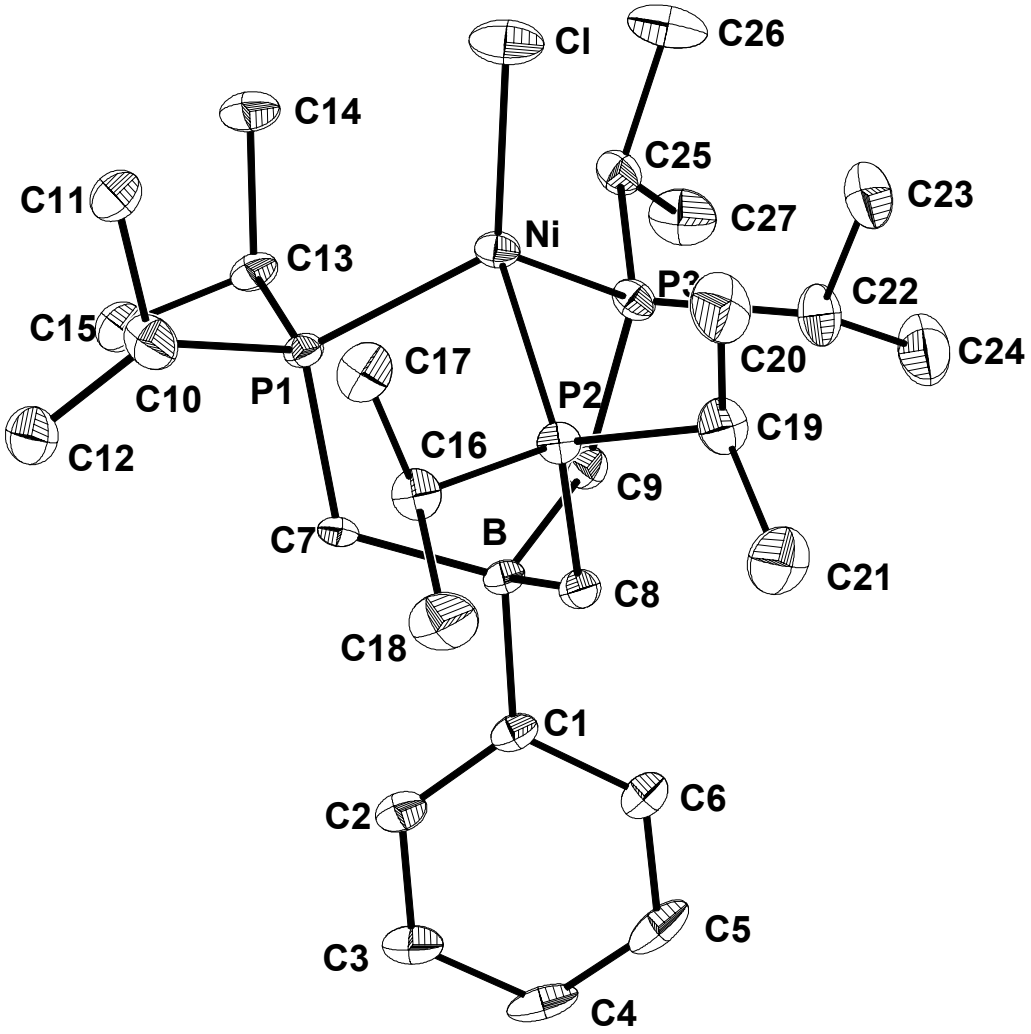


Table 7. Crystal data and structure refinement for $[PhB(CH_2P^iPr_2)_3]NiCl$ (3).

Empirical formula	$C_{27}H_{53}BClNiP_3$	
Formula weight	575.57	
Crystal Habit	Irregular column	
Crystal Color	Pale lime green	
Crystal size	0.07 x 0.15 x 0.37 mm^3	
Data Collection		
Type of diffractometer	CCD area detector	
Wavelength	0.71073 Å	
Data collection temperature	100(2) K	
Unit cell dimensions	a = 9.4015(8) Å	$\alpha = 90°$
	b = 11.5998(10) Å	$\beta = 90°$
	c = 29.392(3) Å	$\gamma = 90°$
Volume	3205.4(5) $Å^3$	
Z	4	
Crystal system	Orthorhombic	
Space group	$P2_12_12_1$	
Density (calculated)	1.193 Mg/m^3	
F(000)	1240	
θ range for data collection	1.39 to 28.44°	
Completeness to θ = 28.44°	90.6%	
Index ranges	$-11 \le h \le 12$, $-7 \le k \le 15$, $-33 \le l \le 39$	
Reflections collected	11806	
Independent reflections	6851 [R(int) = 0.0430]	
Absorption coefficient	0.852 mm^{-1}	
Absorption correction	None	
Structure solution and refinement		
Structure solution program	SHELXS-97 (Sheldrick, 1990)	
Primary solution method	Direct methods	
Hydrogen placement	Calculated positions	
Structure refinement program	SHELXL-97 (Sheldrick, 1997)	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	6851 / 0 / 311	
Goodness-of-fit on F^2	1.133	
Final R indices [$I>2\sigma(I)$]	R1 = 0.0392, wR2 = 0.0717	
R indices (all data)	R1 = 0.0526, wR2 = 0.0751	
Type of weighting scheme used	Calculated	
Weighting scheme used	$w=1/[\sigma^2(F_o^2)+(0.02P)^2]$ where $P=(F_o^2+2F_c^2)/3$	
Max shift/error	0.000	
Average shift/error	0.000	
Absolute structure parameter	0.521(13)	
Largest diff. peak and hole	0.592 and -0.311 $e \cdot Å^{-3}$	

Special refinement details: The crystal was refined as a chiral twin.

Table 8. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for 3. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
Ni	-141(1)	5397(1)	920(1)	16(1)
P(1)	-227(1)	6128(1)	1643(1)	14(1)
P(2)	2253(1)	5697(1)	842(1)	16(1)
P(3)	78(1)	3532(1)	1157(1)	16(1)
Cl	-1637(1)	5798(1)	378(1)	36(1)
B	2267(3)	4582(3)	1757(1)	14(1)
C(1)	3437(3)	4163(2)	2137(1)	16(1)
C(2)	3618(3)	4665(3)	2563(1)	21(1)
C(3)	4637(3)	4298(3)	2878(1)	27(1)
C(4)	5514(3)	3376(3)	2774(1)	30(1)
C(5)	5364(3)	2844(3)	2354(1)	29(1)
C(6)	4347(3)	3221(3)	2048(1)	21(1)
C(7)	1371(3)	5717(3)	1955(1)	13(1)
C(8)	3197(3)	4946(3)	1295(1)	16(1)
C(9)	1173(3)	3468(2)	1664(1)	17(1)
C(10)	-370(4)	7730(2)	1649(1)	31(1)
C(11)	-1638(4)	8170(3)	1387(1)	30(1)
C(12)	-19(5)	8362(3)	2072(1)	40(1)
C(13)	-1713(3)	5519(3)	1980(1)	17(1)
C(14)	-3139(3)	5558(3)	1720(1)	25(1)
C(15)	-1906(3)	6022(3)	2456(1)	26(1)
C(16)	2678(3)	7250(2)	926(1)	21(1)
C(17)	1724(3)	8031(3)	637(1)	27(1)
C(18)	4252(3)	7607(3)	869(2)	37(1)
C(19)	3016(3)	5209(3)	293(1)	25(1)
C(20)	2332(4)	5775(3)	-121(1)	39(1)
C(21)	4640(3)	5219(3)	264(1)	38(1)
C(22)	1021(4)	2641(3)	726(1)	25(1)
C(23)	447(4)	2809(3)	247(1)	33(1)
C(24)	1259(4)	1371(3)	841(1)	42(1)
C(25)	-1641(3)	2828(3)	1301(1)	19(1)
C(26)	-2635(4)	2728(3)	889(1)	36(1)
C(27)	-1539(4)	1686(3)	1558(1)	32(1)

Table 9. Selected bond lengths [Å] and angles [°] for 3.

Ni-Cl	2.1772(9)	Cl-Ni-P(3)	118.94(3)
Ni-P(3)	2.2811(8)	Cl-Ni-P(1)	125.30(4)
Ni-P(1)	2.2871(8)	Cl-Ni-P(2)	121.92(4)
Ni-P(2)	2.2893(9)	P(3)-Ni-P(1)	94.16(3)
Ni-B	3.474(3)	P(3)-Ni-P(2)	94.97(3)
		P(1)-Ni-P(2)	94.12(3)

Table 10. Bond lengths [Å] and angles [°] for 3.

Ni-Cl	2.1772(9)	C(17)-H(17A)	0.9800
Ni-P(3)	2.2811(8)	C(17)-H(17B)	0.9800
Ni-P(1)	2.2871(8)	C(17)-H(17C)	0.9800
Ni-P(2)	2.2893(9)	C(18)-H(18A)	0.9800
Ni-B	3.474(3)	C(18)-H(18B)	0.9800
P(1)-C(7)	1.823(3)	C(18)-H(18C)	0.9800
P(1)-C(13)	1.853(3)	C(19)-C(20)	1.523(4)
P(1)-C(10)	1.864(3)	C(19)-C(21)	1.529(4)
P(2)-C(8)	1.821(3)	C(19)-H(19)	1.0000
P(2)-C(19)	1.856(3)	C(20)-H(20A)	0.9800
P(2)-C(16)	1.861(3)	C(20)-H(20B)	0.9800
P(3)-C(9)	1.815(3)	C(20)-H(20C)	0.9800
P(3)-C(22)	1.858(3)	C(21)-H(21A)	0.9800
P(3)-C(25)	1.860(3)	C(21)-H(21B)	0.9800
B-C(1)	1.641(4)	C(21)-H(21C)	0.9800
B-C(7)	1.667(4)	C(22)-C(23)	1.521(5)
B-C(8)	1.671(4)	C(22)-C(24)	1.528(5)
B-C(9)	1.674(4)	C(22)-H(22)	1.0000
C(1)-C(2)	1.390(4)	C(23)-H(23A)	0.9800
C(1)-C(6)	1.413(4)	C(23)-H(23B)	0.9800
C(2)-C(3)	1.400(4)	C(23)-H(23C)	0.9800
C(2)-H(2)	0.9500	C(24)-H(24A)	0.9800
C(3)-C(4)	1.385(4)	C(24)-H(24B)	0.9800
C(3)-H(3)	0.9500	C(24)-H(24C)	0.9800
C(4)-C(5)	1.387(5)	C(25)-C(27)	1.527(4)
C(4)-H(4)	0.9500	C(25)-C(26)	1.535(4)
C(5)-C(6)	1.384(4)	C(25)-H(25)	1.0000
C(5)-H(5)	0.9500	C(26)-H(26A)	0.9800
C(6)-H(6)	0.9500	C(26)-H(26B)	0.9800
C(7)-H(7A)	0.9900	C(26)-H(26C)	0.9800
C(7)-H(7B)	0.9900	C(27)-H(27A)	0.9800
C(8)-H(8A)	0.9900	C(27)-H(27B)	0.9800
C(8)-H(8B)	0.9900	C(27)-H(27C)	0.9800
C(9)-H(9A)	0.9900		
C(9)-H(9B)	0.9900	Cl-Ni-P(3)	118.94(3)
C(10)-C(12)	1.479(4)	Cl-Ni-P(1)	125.30(4)
C(10)-C(11)	1.508(4)	P(3)-Ni-P(1)	94.16(3)
C(10)-H(10)	1.0000	Cl-Ni-P(2)	121.92(4)
C(11)-H(11A)	0.9800	P(3)-Ni-P(2)	94.97(3)
C(11)-H(11B)	0.9800	P(1)-Ni-P(2)	94.12(3)
C(11)-H(11C)	0.9800	Cl-Ni-B	176.37(6)
C(12)-H(12A)	0.9800	P(3)-Ni-B	57.85(6)
C(12)-H(12B)	0.9800	P(1)-Ni-B	57.77(6)
C(12)-H(12C)	0.9800	P(2)-Ni-B	58.15(6)
C(13)-C(15)	1.529(4)	C(7)-P(1)-C(13)	104.63(12)
C(13)-C(14)	1.543(4)	C(7)-P(1)-C(10)	108.36(15)
C(13)-H(13)	1.0000	C(13)-P(1)-C(10)	108.66(16)
C(14)-H(14A)	0.9800	C(7)-P(1)-Ni	109.93(10)
C(14)-H(14B)	0.9800	C(13)-P(1)-Ni	112.41(10)
C(14)-H(14C)	0.9800	C(10)-P(1)-Ni	112.47(11)
C(15)-H(15A)	0.9800	C(8)-P(2)-C(19)	107.53(15)
C(15)-H(15B)	0.9800	C(8)-P(2)-C(16)	105.20(15)
C(15)-H(15C)	0.9800	C(19)-P(2)-C(16)	109.14(15)
C(16)-C(17)	1.531(4)	C(8)-P(2)-Ni	109.42(10)
C(16)-C(18)	1.546(4)	C(19)-P(2)-Ni	114.90(11)
C(16)-H(16)	1.0000	C(16)-P(2)-Ni	110.18(10)

C(9)-P(3)-C(22)	105.45(15)	C(10)-C(11)-H(11A)	109.5
C(9)-P(3)-C(25)	106.70(14)	C(10)-C(11)-H(11B)	109.5
C(22)-P(3)-C(25)	109.02(15)	H(11A)-C(11)-H(11B)	109.5
C(9)-P(3)-Ni	109.87(10)	C(10)-C(11)-H(11C)	109.5
C(22)-P(3)-Ni	111.29(11)	H(11A)-C(11)-H(11C)	109.5
C(25)-P(3)-Ni	114.06(10)	H(11B)-C(11)-H(11C)	109.5
C(1)-B-C(7)	109.6(2)	C(10)-C(12)-H(12A)	109.5
C(1)-B-C(8)	106.1(2)	C(10)-C(12)-H(12B)	109.5
C(7)-B-C(8)	110.4(2)	H(12A)-C(12)-H(12B)	109.5
C(1)-B-C(9)	107.1(2)	C(10)-C(12)-H(12C)	109.5
C(7)-B-C(9)	110.9(2)	H(12A)-C(12)-H(12C)	109.5
C(8)-B-C(9)	112.5(2)	H(12B)-C(12)-H(12C)	109.5
C(1)-B-Ni	177.6(2)	C(15)-C(13)-C(14)	109.8(3)
C(7)-B-Ni	72.69(15)	C(15)-C(13)-P(1)	115.7(2)
C(8)-B-Ni	72.30(15)	C(14)-C(13)-P(1)	112.3(2)
C(9)-B-Ni	72.19(15)	C(15)-C(13)-H(13)	106.1
C(2)-C(1)-C(6)	114.6(3)	C(14)-C(13)-H(13)	106.1
C(2)-C(1)-B	124.8(3)	P(1)-C(13)-H(13)	106.1
C(6)-C(1)-B	120.6(3)	C(13)-C(14)-H(14A)	109.5
C(1)-C(2)-C(3)	123.6(3)	C(13)-C(14)-H(14B)	109.5
C(1)-C(2)-H(2)	118.2	H(14A)-C(14)-H(14B)	109.5
C(3)-C(2)-H(2)	118.2	C(13)-C(14)-H(14C)	109.5
C(4)-C(3)-C(2)	119.7(3)	H(14A)-C(14)-H(14C)	109.5
C(4)-C(3)-H(3)	120.1	H(14B)-C(14)-H(14C)	109.5
C(2)-C(3)-H(3)	120.1	C(13)-C(15)-H(15A)	109.5
C(3)-C(4)-C(5)	118.7(3)	C(13)-C(15)-H(15B)	109.5
C(3)-C(4)-H(4)	120.7	H(15A)-C(15)-H(15B)	109.5
C(5)-C(4)-H(4)	120.7	C(13)-C(15)-H(15C)	109.5
C(6)-C(5)-C(4)	120.5(3)	H(15A)-C(15)-H(15C)	109.5
C(6)-C(5)-H(5)	119.7	H(15B)-C(15)-H(15C)	109.5
C(4)-C(5)-H(5)	119.7	C(17)-C(16)-C(18)	110.0(3)
C(5)-C(6)-C(1)	122.9(3)	C(17)-C(16)-P(2)	111.9(2)
C(5)-C(6)-H(6)	118.6	C(18)-C(16)-P(2)	116.7(2)
C(1)-C(6)-H(6)	118.6	C(17)-C(16)-H(16)	105.8
B-C(7)-P(1)	116.6(2)	C(18)-C(16)-H(16)	105.8
B-C(7)-H(7A)	108.1	P(2)-C(16)-H(16)	105.8
P(1)-C(7)-H(7A)	108.1	C(16)-C(17)-H(17A)	109.5
B-C(7)-H(7B)	108.1	C(16)-C(17)-H(17B)	109.5
P(1)-C(7)-H(7B)	108.1	H(17A)-C(17)-H(17B)	109.5
H(7A)-C(7)-H(7B)	107.3	C(16)-C(17)-H(17C)	109.5
B-C(8)-P(2)	117.40(19)	H(17A)-C(17)-H(17C)	109.5
B-C(8)-H(8A)	108.0	H(17B)-C(17)-H(17C)	109.5
P(2)-C(8)-H(8A)	108.0	C(16)-C(18)-H(18A)	109.5
B-C(8)-H(8B)	108.0	C(16)-C(18)-H(18B)	109.5
P(2)-C(8)-H(8B)	108.0	H(18A)-C(18)-H(18B)	109.5
H(8A)-C(8)-H(8B)	107.2	C(16)-C(18)-H(18C)	109.5
B-C(9)-P(3)	116.8(2)	H(18A)-C(18)-H(18C)	109.5
B-C(9)-H(9A)	108.1	H(18B)-C(18)-H(18C)	109.5
P(3)-C(9)-H(9A)	108.1	C(20)-C(19)-C(21)	111.9(3)
B-C(9)-H(9B)	108.1	C(20)-C(19)-P(2)	113.5(2)
P(3)-C(9)-H(9B)	108.1	C(21)-C(19)-P(2)	115.6(2)
H(9A)-C(9)-H(9B)	107.3	C(20)-C(19)-H(19)	104.8
C(12)-C(10)-C(11)	116.0(3)	C(21)-C(19)-H(19)	104.8
C(12)-C(10)-P(1)	119.1(2)	P(2)-C(19)-H(19)	104.8
C(11)-C(10)-P(1)	112.9(2)	C(19)-C(20)-H(20A)	109.5
C(12)-C(10)-H(10)	101.7	C(19)-C(20)-H(20B)	109.5
C(11)-C(10)-H(10)	101.7	H(20A)-C(20)-H(20B)	109.5
P(1)-C(10)-H(10)	101.7	C(19)-C(20)-H(20C)	109.5

H(20A)-C(20)-H(20C)	109.5	H(24A)-C(24)-H(24B)	109.5
H(20B)-C(20)-H(20C)	109.5	C(22)-C(24)-H(24C)	109.5
C(19)-C(21)-H(21A)	109.5	H(24A)-C(24)-H(24C)	109.5
C(19)-C(21)-H(21B)	109.5	H(24B)-C(24)-H(24C)	109.5
H(21A)-C(21)-H(21B)	109.5	C(27)-C(25)-C(26)	111.3(3)
C(19)-C(21)-H(21C)	109.5	C(27)-C(25)-P(3)	116.1(2)
H(21A)-C(21)-H(21C)	109.5	C(26)-C(25)-P(3)	112.4(2)
H(21B)-C(21)-H(21C)	109.5	C(27)-C(25)-H(25)	105.3
C(23)-C(22)-C(24)	112.2(3)	C(26)-C(25)-H(25)	105.3
C(23)-C(22)-P(3)	113.0(2)	P(3)-C(25)-H(25)	105.3
C(24)-C(22)-P(3)	117.2(2)	C(25)-C(26)-H(26A)	109.5
C(23)-C(22)-H(22)	104.3	C(25)-C(26)-H(26B)	109.5
C(24)-C(22)-H(22)	104.3	H(26A)-C(26)-H(26B)	109.5
P(3)-C(22)-H(22)	104.3	C(25)-C(26)-H(26C)	109.5
C(22)-C(23)-H(23A)	109.5	H(26A)-C(26)-H(26C)	109.5
C(22)-C(23)-H(23B)	109.5	H(26B)-C(26)-H(26C)	109.5
H(23A)-C(23)-H(23B)	109.5	C(25)-C(27)-H(27A)	109.5
C(22)-C(23)-H(23C)	109.5	C(25)-C(27)-H(27B)	109.5
H(23A)-C(23)-H(23C)	109.5	H(27A)-C(27)-H(27B)	109.5
H(23B)-C(23)-H(23C)	109.5	C(25)-C(27)-H(27C)	109.5
C(22)-C(24)-H(24A)	109.5	H(27A)-C(27)-H(27C)	109.5
C(22)-C(24)-H(24B)	109.5	H(27B)-C(27)-H(27C)	109.5

Table 11. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for 3. The anisotropic displacement factor exponent takes the form: $-2\pi^2[\ h^2\ a^{*2}U^{11} + ...\ + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Ni	15(1)	16(1)	15(1)	3(1)	-3(1)	-2(1)
P(1)	12(1)	12(1)	18(1)	1(1)	-2(1)	1(1)
P(2)	17(1)	16(1)	16(1)	3(1)	1(1)	-1(1)
P(3)	19(1)	14(1)	15(1)	1(1)	-2(1)	-3(1)
Cl	33(1)	45(1)	29(1)	12(1)	-15(1)	-1(1)
B	12(2)	15(2)	15(2)	3(1)	-2(1)	1(1)
C(1)	11(1)	15(1)	21(2)	6(1)	1(1)	-1(1)
C(2)	14(2)	23(2)	25(2)	3(2)	-1(1)	-1(1)
C(3)	21(2)	34(2)	28(2)	3(2)	-10(2)	1(1)
C(4)	16(2)	38(2)	36(2)	16(2)	-8(2)	4(1)
C(5)	18(2)	24(2)	45(2)	13(2)	4(2)	9(1)
C(6)	18(2)	20(2)	25(2)	3(2)	1(1)	4(1)
C(7)	10(1)	16(2)	14(2)	0(1)	-3(1)	-2(1)
C(8)	15(2)	16(1)	18(2)	1(1)	-1(1)	0(1)
C(9)	17(2)	15(1)	19(2)	1(1)	1(1)	1(1)
C(10)	44(2)	14(1)	34(2)	1(1)	-14(2)	2(2)
C(11)	31(2)	24(2)	35(2)	0(2)	-8(2)	10(2)
C(12)	44(2)	25(2)	51(2)	-10(2)	-14(2)	9(2)
C(13)	11(1)	18(2)	23(2)	3(1)	1(1)	-1(1)
C(14)	16(2)	28(2)	32(2)	5(2)	-5(2)	-4(1)
C(15)	17(2)	35(2)	27(2)	-5(2)	6(2)	1(1)
C(16)	24(2)	17(1)	22(2)	4(1)	3(2)	-4(1)
C(17)	29(2)	20(2)	31(2)	7(2)	6(2)	-2(1)
C(18)	29(2)	24(2)	59(3)	6(2)	-4(2)	-11(1)
C(19)	29(2)	26(2)	21(2)	1(2)	6(2)	-2(1)
C(20)	54(2)	46(2)	16(2)	3(2)	5(2)	6(2)
C(21)	33(2)	49(2)	34(2)	0(2)	14(2)	-1(2)
C(22)	34(2)	23(2)	19(2)	-1(2)	9(2)	-1(1)
C(23)	45(2)	29(2)	25(2)	-6(2)	4(2)	1(2)
C(24)	54(2)	33(2)	38(2)	-9(2)	0(2)	5(2)
C(25)	22(2)	16(2)	20(2)	-1(1)	-2(2)	-4(1)
C(26)	29(2)	47(2)	32(2)	11(2)	-13(2)	-16(2)
C(27)	30(2)	27(2)	38(2)	9(2)	-1(2)	-12(2)

Table 12. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for 3.

	x	y	z	U(eq)
H(2)	3018	5292	2643	25
H(3)	4725	4679	3163	33
H(4)	6205	3114	2986	36
H(5)	5964	2216	2276	35
H(6)	4258	2830	1766	25
H(7A)	2023	6387	1959	16
H(7B)	1096	5555	2274	16
H(8A)	3609	4233	1164	20
H(8B)	4001	5438	1393	20
H(9A)	536	3393	1931	20
H(9B)	1756	2758	1649	20
H(10)	434	7958	1446	37
H(11A)	-2503	8056	1567	45
H(11B)	-1720	7746	1099	45
H(11C)	-1514	8993	1323	45
H(12A)	173	9172	1999	60
H(12B)	824	8017	2212	60
H(12C)	-823	8315	2283	60
H(13)	-1487	4684	2023	21
H(14A)	-3842	5081	1878	38
H(14B)	-3000	5263	1410	38
H(14C)	-3480	6356	1705	38
H(15A)	-2299	6803	2433	39
H(15B)	-984	6052	2611	39
H(15C)	-2561	5535	2631	39
H(16)	2431	7425	1249	25
H(17A)	1772	8822	753	40
H(17B)	740	7755	653	40
H(17C)	2049	8015	320	40
H(18A)	4479	7668	544	56
H(18B)	4866	7026	1010	56
H(18C)	4409	8355	1016	56
H(19)	2748	4377	270	30
H(20A)	2657	6576	-144	58
H(20B)	1295	5760	-88	58
H(20C)	2604	5353	-396	58
H(21A)	4945	4795	-8	57
H(21B)	5039	4852	535	57
H(21C)	4977	6017	245	57
H(22)	2001	2976	715	30
H(23A)	1107	2466	28	49
H(23B)	347	3635	184	49
H(23C)	-484	2435	221	49
H(24A)	368	945	799	62
H(24B)	1572	1300	1157	62
H(24C)	1990	1053	639	62
H(25)	-2127	3370	1515	23
H(26A)	-2328	2084	696	54
H(26B)	-2601	3445	713	54
H(26C)	-3610	2591	993	54
H(27A)	-2495	1429	1644	47
H(27B)	-962	1791	1832	47
H(27C)	-1095	1105	1362	47

Figure 3. Fully-labeled displacement ellipsoid (50%) representation of (0.84)[$PhB(CH_2PPh_2)_3$]Ni(N_3) · (0.16)$C_{45}H_{41}BClNiP_3$ (**(0.84)4 · (0.16)1**) (hydrogens and chloride position omitted for clarity).

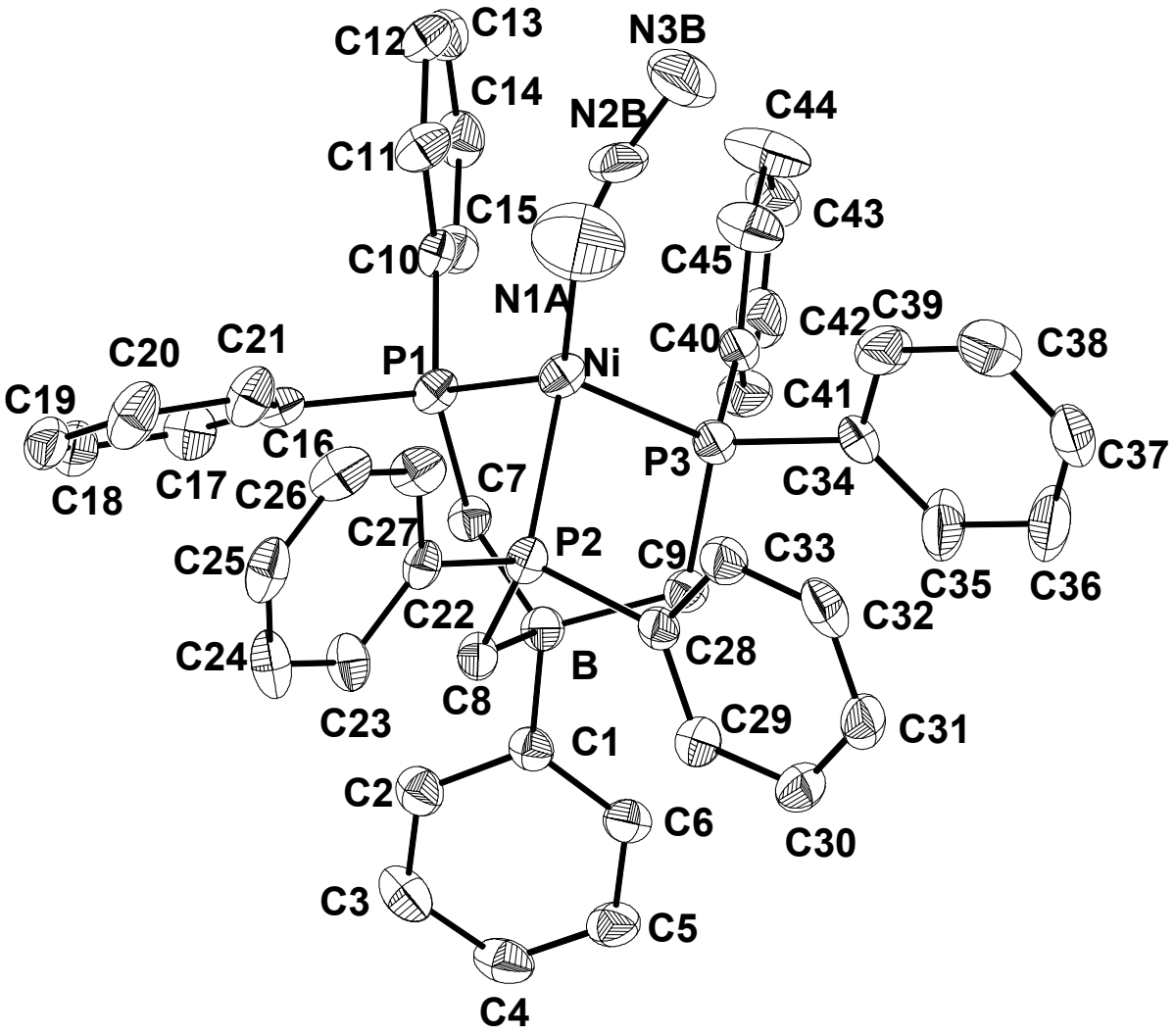


Table 13. Crystal data and structure refinement for (0.84)4 · (0.16)1.

Empirical formula	$(0.84)C_{45}H_{41}BN_3NiP_3 \cdot (0.16)C_{45}H_{41}BClNiP_3$	
Moiety formula	$(0.84)C_{45}H_{41}BN_3NiP_3 \cdot (0.16)C_{45}H_{41}BClNiP_3$	
Formula weight	821.69	
Crystal habit	plate	
Crystal color	yellow-green	
Crystal size	0.16 x 0.28 x 0.30 mm^3	
Data Collection		
Type of diffractometer	CCD area detector	
Wavelength	0.71073 Å	
Temperature	98(2) K	
Unit cell dimensions	a = 40.37(3) Å	α = 90°
	b = 12.887(15) Å	β = 111.48(6)°
	c = 16.067(12) Å	γ = 90°
Volume	7779(13) $Å^3$	
Z	8	
Crystal system	Monoclinic	
Space group	C2/c	
Density (calculated)	1.403 g/cm^3	
F(000)	3416	
θ range for data collection	1.67 to 28.41°	
Completeness to θ = 28.41°	84.4%	
Index ranges	$-35 \le h \le 50$, $-7 \le k \le 16$, $-21 \le l \le 21$	
Reflections collected	19273	
Independent reflections	8264 [R(int) = 0.0668]	
Absorption coefficient	0.729 mm^{-1}	
Absorption correction	None	
Structure solution and refinement		
Structure solution program	SHELXS-97 (Sheldrick, 1990)	
Primary solution method	direct methods	
Secondary solution method	difference Fourier map	
Hydrogen placement	Calculated positions	
Structure refinement program	SHELXL-97 (Sheldrick, 1997)	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	8264 / 1 / 508	
Goodness-of-fit on F^2	1.139	
Final R indices [$I>2\sigma(I)$]	R1 = 0.0489, wR2 = 0.0708	
R indices (all data)	R1 = 0.0963, wR2 = 0.0781	
Type of weighting scheme used	calculated	
Weighting scheme used	$w=1/[\sigma^2(F_o^2)]$	
Max shift/error	0.001	
Average shift/error	0.000	
Largest diff. peak and hole	0.673 and -0.654 $e \cdot Å^{-3}$	

Additional refinement details: The structure contained a mixture of the azide (majority) and chloride (minority) nickel complexes. The chloride position was assigned and refined at 0.16 occupancy to provide the final structure.

Table 14. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$ x 10^3) for (0.84)4 · (0.16)1. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
Ni	987(1)	2842(1)	3162(1)	28(1)
P(1)	1491(1)	3749(1)	3871(1)	26(1)
P(2)	907(1)	3463(1)	1786(1)	26(1)
P(3)	1305(1)	1484(1)	2977(1)	27(1)
N(1A)	593(3)	2675(9)	3544(7)	96(6)
Cl	563(4)	2630(13)	3671(11)	36(3)
N(2A)	338(3)	1921(6)	3231(6)	50(2)
N(3A)	98(2)	1365(6)	3018(6)	77(3)
N(2B)	544(3)	2227(12)	3995(10)	40(3)
N(3B)	442(2)	1597(6)	4386(6)	71(4)
B	1675(1)	3097(2)	2342(2)	25(1)
C(1)	1982(1)	3242(2)	1931(2)	24(1)
C(2)	2151(1)	4199(2)	1977(2)	31(1)
C(3)	2416(1)	4360(2)	1633(2)	39(1)
C(4)	2525(1)	3561(2)	1213(2)	36(1)
C(5)	2361(1)	2624(2)	1133(2)	35(1)
C(6)	2093(1)	2464(2)	1478(2)	30(1)
C(7)	1829(1)	3498(2)	3402(2)	24(1)
C(8)	1327(1)	3850(2)	1738(2)	27(1)
C(9)	1556(1)	1844(2)	2299(2)	26(1)
C(10)	1659(1)	3463(2)	5071(2)	24(1)
C(11)	1418(1)	3527(2)	5501(2)	32(1)
C(12)	1521(1)	3291(2)	6402(2)	37(1)
C(13)	1864(1)	2974(2)	6877(2)	35(1)
C(14)	2105(1)	2897(2)	6463(2)	35(1)
C(15)	2005(1)	3146(2)	5558(2)	31(1)
C(16)	1420(1)	5153(2)	3820(2)	26(1)
C(17)	1703(1)	5845(2)	4128(2)	35(1)
C(18)	1646(1)	6895(2)	4044(2)	39(1)
C(19)	1302(1)	7278(2)	3639(2)	37(1)
C(20)	1020(1)	6605(2)	3361(2)	45(1)
C(21)	1081(1)	5540(2)	3459(2)	35(1)
C(22)	581(1)	4515(2)	1415(2)	26(1)
C(23)	613(1)	5287(2)	846(2)	33(1)
C(24)	363(1)	6067(2)	567(2)	39(1)
C(25)	74(1)	6084(2)	838(2)	37(1)
C(26)	38(1)	5322(3)	1393(2)	39(1)
C(27)	292(1)	4539(2)	1680(2)	35(1)
C(28)	717(1)	2497(2)	914(2)	24(1)
C(29)	850(1)	2269(2)	259(2)	33(1)
C(30)	688(1)	1520(2)	-387(2)	38(1)
C(31)	393(1)	1008(2)	-392(2)	39(1)
C(32)	250(1)	1232(2)	250(2)	39(1)
C(33)	413(1)	1964(2)	906(2)	32(1)
C(34)	1032(1)	348(2)	2475(2)	28(1)
C(35)	1111(1)	-290(3)	1892(3)	63(1)
C(36)	893(1)	-1118(3)	1499(3)	70(1)
C(37)	597(1)	-1325(2)	1690(2)	41(1)
C(38)	518(1)	-701(3)	2280(2)	46(1)
C(39)	737(1)	128(3)	2673(2)	42(1)
C(40)	1622(1)	994(2)	4040(2)	28(1)
C(41)	1981(1)	856(2)	4215(2)	35(1)
C(42)	2207(1)	503(2)	5039(2)	39(1)

C(43)	2083(1)	275(2)	5698(2)	42(1)
C(44)	1727(1)	409(3)	5538(2)	62(1)
C(45)	1499(1)	768(2)	4718(2)	44(1)

Table 15. Selected bond lengths [Å] and angles [°] for (0.84)4 · (0.16)1.

Ni-N(1A)	1.915(12)
Ni-Cl	2.17(2)
Ni-P(3)	2.255(2)
Ni-P(2)	2.2609(18)
Ni-P(1)	2.262(2)
N(1A)-Ni-P(3)	122.4(4)
N(1A)-Ni-P(2)	121.1(3)
P(3)-Ni-P(2)	91.67(6)
N(1A)-Ni-P(1)	126.7(4)
P(3)-Ni-P(1)	90.90(8)
P(2)-Ni-P(1)	95.09(7)

Table 16. Bond lengths [Å] and angles [°] for (0.84)4 · (0.16)1.

Ni-N(1A)	1.915(12)	C(18)-H(18)	0.9500
Ni-Cl	2.17(2)	C(19)-C(20)	1.368(4)
Ni-P(3)	2.255(2)	C(19)-H(19)	0.9500
Ni-P(2)	2.2609(18)	C(20)-C(21)	1.394(4)
Ni-P(1)	2.262(2)	C(20)-H(20)	0.9500
P(1)-C(7)	1.814(3)	C(21)-H(21)	0.9500
P(1)-C(16)	1.828(4)	C(22)-C(27)	1.384(4)
P(1)-C(10)	1.831(3)	C(22)-C(23)	1.388(4)
P(2)-C(8)	1.797(3)	C(23)-C(24)	1.379(4)
P(2)-C(28)	1.820(3)	C(23)-H(23)	0.9500
P(2)-C(22)	1.830(3)	C(24)-C(25)	1.385(4)
P(3)-C(9)	1.798(3)	C(24)-H(24)	0.9500
P(3)-C(40)	1.830(3)	C(25)-C(26)	1.369(4)
P(3)-C(34)	1.832(3)	C(25)-H(25)	0.9500
N(1A)-N(2B)	1.00(2)	C(26)-C(27)	1.390(4)
N(1A)-N(2A)	1.369(13)	C(26)-H(26)	0.9500
N(2A)-N(3A)	1.151(11)	C(27)-H(27)	0.9500
N(3A)-N(3A)#1	1.560(18)	C(28)-C(29)	1.378(4)
N(2B)-N(3B)	1.187(15)	C(28)-C(33)	1.401(4)
B-C(1)	1.614(4)	C(29)-C(30)	1.392(4)
B-C(7)	1.667(4)	C(29)-H(29)	0.9500
B-C(9)	1.679(4)	C(30)-C(31)	1.360(4)
B-C(8)	1.692(4)	C(30)-H(30)	0.9500
C(1)-C(2)	1.398(4)	C(31)-C(32)	1.384(4)
C(1)-C(6)	1.405(4)	C(31)-H(31)	0.9500
C(2)-C(3)	1.388(4)	C(32)-C(33)	1.388(4)
C(2)-H(2)	0.9500	C(32)-H(32)	0.9500
C(3)-C(4)	1.389(4)	C(33)-H(33)	0.9500
C(3)-H(3)	0.9500	C(34)-C(39)	1.368(4)
C(4)-C(5)	1.361(4)	C(34)-C(35)	1.369(4)
C(4)-H(4)	0.9500	C(35)-C(36)	1.379(5)
C(5)-C(6)	1.398(4)	C(35)-H(35)	0.9500
C(5)-H(5)	0.9500	C(36)-C(37)	1.364(4)
C(6)-H(6)	0.9500	C(36)-H(36)	0.9500
C(7)-H(7A)	0.9900	C(37)-C(38)	1.366(4)
C(7)-H(7B)	0.9900	C(37)-H(37)	0.9500
C(8)-H(8A)	0.9900	C(38)-C(39)	1.384(4)
C(8)-H(8B)	0.9900	C(38)-H(38)	0.9500
C(9)-H(9A)	0.9900	C(39)-H(39)	0.9500
C(9)-H(9B)	0.9900	C(40)-C(45)	1.382(4)
C(10)-C(11)	1.386(4)	C(40)-C(41)	1.384(4)
C(10)-C(15)	1.391(4)	C(41)-C(42)	1.383(4)
C(11)-C(12)	1.386(4)	C(41)-H(41)	0.9500
C(11)-H(11)	0.9500	C(42)-C(43)	1.361(4)
C(12)-C(13)	1.374(4)	C(42)-H(42)	0.9500
C(12)-H(12)	0.9500	C(43)-C(44)	1.372(5)
C(13)-C(14)	1.370(4)	C(43)-H(43)	0.9500
C(13)-H(13)	0.9500	C(44)-C(45)	1.382(5)
C(14)-C(15)	1.396(4)	C(44)-H(44)	0.9500
C(14)-H(14)	0.9500	C(45)-H(45)	0.9500
C(15)-H(15)	0.9500		
C(16)-C(21)	1.372(4)	N(1A)-Ni-Cl	3.3(6)
C(16)-C(17)	1.390(4)	N(1A)-Ni-P(3)	122.4(4)
C(17)-C(18)	1.371(4)	Cl-Ni-P(3)	121.3(4)
C(17)-H(17)	0.9500	N(1A)-Ni-P(2)	121.1(3)
C(18)-C(19)	1.390(4)	Cl-Ni-P(2)	124.4(4)

P(3)-Ni-P(2)	91.67(6)	H(7A)-C(7)-H(7B)	107.5
N(1A)-Ni-P(1)	126.7(4)	B-C(8)-P(2)	114.5(2)
Cl-Ni-P(1)	124.4(4)	B-C(8)-H(8A)	108.6
P(3)-Ni-P(1)	90.90(8)	P(2)-C(8)-H(8A)	108.6
P(2)-Ni-P(1)	95.09(7)	B-C(8)-H(8B)	108.6
C(7)-P(1)-C(16)	106.68(13)	P(2)-C(8)-H(8B)	108.6
C(7)-P(1)-C(10)	110.97(15)	H(8A)-C(8)-H(8B)	107.6
C(16)-P(1)-C(10)	103.77(12)	B-C(9)-P(3)	116.09(18)
C(7)-P(1)-Ni	111.99(11)	B-C(9)-H(9A)	108.3
C(16)-P(1)-Ni	113.04(12)	P(3)-C(9)-H(9A)	108.3
C(10)-P(1)-Ni	110.06(11)	B-C(9)-H(9B)	108.3
C(8)-P(2)-C(28)	107.16(14)	P(3)-C(9)-H(9B)	108.3
C(8)-P(2)-C(22)	110.87(15)	H(9A)-C(9)-H(9B)	107.4
C(28)-P(2)-C(22)	101.86(15)	C(11)-C(10)-C(15)	118.8(3)
C(8)-P(2)-Ni	110.01(11)	C(11)-C(10)-P(1)	117.2(2)
C(28)-P(2)-Ni	112.35(11)	C(15)-C(10)-P(1)	124.0(2)
C(22)-P(2)-Ni	114.16(11)	C(12)-C(11)-C(10)	120.7(3)
C(9)-P(3)-C(40)	107.40(15)	C(12)-C(11)-H(11)	119.7
C(9)-P(3)-C(34)	108.72(14)	C(10)-C(11)-H(11)	119.7
C(40)-P(3)-C(34)	103.78(14)	C(13)-C(12)-C(11)	120.1(3)
C(9)-P(3)-Ni	110.77(11)	C(13)-C(12)-H(12)	120.0
C(40)-P(3)-Ni	112.38(11)	C(11)-C(12)-H(12)	120.0
C(34)-P(3)-Ni	113.40(13)	C(14)-C(13)-C(12)	120.2(3)
N(2B)-N(1A)-N(2A)	62.4(10)	C(14)-C(13)-H(13)	119.9
N(2B)-N(1A)-Ni	134.7(12)	C(12)-C(13)-H(13)	119.9
N(2A)-N(1A)-Ni	124.2(8)	C(13)-C(14)-C(15)	120.2(3)
N(3A)-N(2A)-N(1A)	170.9(9)	C(13)-C(14)-H(14)	119.9
N(2A)-N(3A)-N(3A)#1	111.1(8)	C(15)-C(14)-H(14)	119.9
N(1A)-N(2B)-N(3B)	167.2(16)	C(10)-C(15)-C(14)	120.0(3)
C(1)-B-C(7)	109.1(2)	C(10)-C(15)-H(15)	120.0
C(1)-B-C(9)	110.3(2)	C(14)-C(15)-H(15)	120.0
C(7)-B-C(9)	109.6(2)	C(21)-C(16)-C(17)	118.8(3)
C(1)-B-C(8)	107.4(2)	C(21)-C(16)-P(1)	119.6(2)
C(7)-B-C(8)	109.2(2)	C(17)-C(16)-P(1)	121.6(2)
C(9)-B-C(8)	111.2(3)	C(18)-C(17)-C(16)	120.7(3)
C(2)-C(1)-C(6)	114.5(3)	C(18)-C(17)-H(17)	119.7
C(2)-C(1)-B	120.8(3)	C(16)-C(17)-H(17)	119.7
C(6)-C(1)-B	124.6(3)	C(17)-C(18)-C(19)	120.1(3)
C(3)-C(2)-C(1)	122.8(3)	C(17)-C(18)-H(18)	120.0
C(3)-C(2)-H(2)	118.6	C(19)-C(18)-H(18)	120.0
C(1)-C(2)-H(2)	118.6	C(20)-C(19)-C(18)	119.8(3)
C(2)-C(3)-C(4)	120.8(3)	C(20)-C(19)-H(19)	120.1
C(2)-C(3)-H(3)	119.6	C(18)-C(19)-H(19)	120.1
C(4)-C(3)-H(3)	119.6	C(19)-C(20)-C(21)	119.8(3)
C(5)-C(4)-C(3)	118.3(3)	C(19)-C(20)-H(20)	120.1
C(5)-C(4)-H(4)	120.9	C(21)-C(20)-H(20)	120.1
C(3)-C(4)-H(4)	120.9	C(16)-C(21)-C(20)	120.8(3)
C(4)-C(5)-C(6)	120.9(3)	C(16)-C(21)-H(21)	119.6
C(4)-C(5)-H(5)	119.6	C(20)-C(21)-H(21)	119.6
C(6)-C(5)-H(5)	119.6	C(27)-C(22)-C(23)	118.6(3)
C(5)-C(6)-C(1)	122.7(3)	C(27)-C(22)-P(2)	120.2(2)
C(5)-C(6)-H(6)	118.7	C(23)-C(22)-P(2)	121.2(2)
C(1)-C(6)-H(6)	118.7	C(24)-C(23)-C(22)	120.2(3)
B-C(7)-P(1)	115.1(2)	C(24)-C(23)-H(23)	119.9
B-C(7)-H(7A)	108.5	C(22)-C(23)-H(23)	119.9
P(1)-C(7)-H(7A)	108.5	C(23)-C(24)-C(25)	120.7(3)
B-C(7)-H(7B)	108.5	C(23)-C(24)-H(24)	119.7
P(1)-C(7)-H(7B)	108.5	C(25)-C(24)-H(24)	119.7

C(26)-C(25)-C(24)	119.6(3)	C(36)-C(35)-H(35)	119.7
C(26)-C(25)-H(25)	120.2	C(37)-C(36)-C(35)	120.7(3)
C(24)-C(25)-H(25)	120.2	C(37)-C(36)-H(36)	119.6
C(25)-C(26)-C(27)	119.8(3)	C(35)-C(36)-H(36)	119.6
C(25)-C(26)-H(26)	120.1	C(36)-C(37)-C(38)	119.2(3)
C(27)-C(26)-H(26)	120.1	C(36)-C(37)-H(37)	120.4
C(22)-C(27)-C(26)	121.1(3)	C(38)-C(37)-H(37)	120.4
C(22)-C(27)-H(27)	119.5	C(37)-C(38)-C(39)	119.9(3)
C(26)-C(27)-H(27)	119.5	C(37)-C(38)-H(38)	120.1
C(29)-C(28)-C(33)	118.3(3)	C(39)-C(38)-H(38)	120.1
C(29)-C(28)-P(2)	124.2(2)	C(34)-C(39)-C(38)	121.2(3)
C(33)-C(28)-P(2)	117.6(2)	C(34)-C(39)-H(39)	119.4
C(28)-C(29)-C(30)	120.6(3)	C(38)-C(39)-H(39)	119.4
C(28)-C(29)-H(29)	119.7	C(45)-C(40)-C(41)	117.6(3)
C(30)-C(29)-H(29)	119.7	C(45)-C(40)-P(3)	118.6(3)
C(31)-C(30)-C(29)	120.8(3)	C(41)-C(40)-P(3)	123.7(2)
C(31)-C(30)-H(30)	119.6	C(42)-C(41)-C(40)	120.9(3)
C(29)-C(30)-H(30)	119.6	C(42)-C(41)-H(41)	119.5
C(30)-C(31)-C(32)	119.8(3)	C(40)-C(41)-H(41)	119.5
C(30)-C(31)-H(31)	120.1	C(43)-C(42)-C(41)	120.8(3)
C(32)-C(31)-H(31)	120.1	C(43)-C(42)-H(42)	119.6
C(31)-C(32)-C(33)	119.8(3)	C(41)-C(42)-H(42)	119.6
C(31)-C(32)-H(32)	120.1	C(42)-C(43)-C(44)	119.1(3)
C(33)-C(32)-H(32)	120.1	C(42)-C(43)-H(43)	120.4
C(32)-C(33)-C(28)	120.6(3)	C(44)-C(43)-H(43)	120.4
C(32)-C(33)-H(33)	119.7	C(43)-C(44)-C(45)	120.5(3)
C(28)-C(33)-H(33)	119.7	C(43)-C(44)-H(44)	119.8
C(39)-C(34)-C(35)	118.3(3)	C(45)-C(44)-H(44)	119.8
C(39)-C(34)-P(3)	119.8(2)	C(40)-C(45)-C(44)	121.1(3)
C(35)-C(34)-P(3)	121.9(3)	C(40)-C(45)-H(45)	119.5
C(34)-C(35)-C(36)	120.6(3)	C(44)-C(45)-H(45)	119.5
C(34)-C(35)-H(35)	119.7		

Symmetry transformations used to generate equivalent atoms:

#1 -x,y,-z+1/2

Table 17. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for (0.84)4 · (0.16)1. The anisotropic displacement factor exponent takes the form: $-2\pi^2[\ h^2 a^{*2} U^{11} + ... + 2\ h\ k\ a^*\ b^*\ U^{12}]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Ni	25(1)	32(1)	27(1)	-3(1)	10(1)	2(1)
P(1)	25(1)	27(1)	24(1)	-3(1)	8(1)	3(1)
P(2)	26(1)	24(1)	25(1)	-3(1)	7(1)	2(1)
P(3)	30(1)	24(1)	30(1)	1(1)	13(1)	0(1)
N(1A)	93(8)	113(8)	79(7)	16(4)	28(4)	5(5)
Cl	24(6)	53(7)	30(5)	6(5)	7(4)	19(5)
N(2A)	52(6)	38(5)	68(7)	5(4)	32(5)	1(4)
N(3A)	45(7)	74(6)	129(8)	-18(5)	52(7)	-26(5)
N(2B)	45(7)	50(7)	36(6)	-7(5)	29(6)	-6(6)
N(3B)	96(8)	55(6)	94(8)	15(5)	71(7)	0(5)
B	27(2)	23(2)	27(2)	3(2)	11(2)	6(2)
C(1)	23(2)	24(2)	25(2)	5(1)	7(1)	6(1)
C(2)	31(2)	27(2)	38(2)	5(2)	16(2)	6(2)
C(3)	36(2)	33(2)	50(2)	12(2)	18(2)	1(2)
C(4)	33(2)	43(2)	39(2)	14(2)	20(2)	10(2)
C(5)	41(2)	35(2)	35(2)	5(2)	22(2)	12(2)
C(6)	33(2)	30(2)	29(2)	2(1)	14(2)	0(2)
C(7)	20(2)	24(2)	31(2)	-1(1)	11(2)	4(1)
C(8)	31(2)	21(2)	30(2)	-2(1)	11(2)	-1(1)
C(9)	27(2)	25(2)	28(2)	1(1)	13(2)	4(1)
C(10)	25(2)	19(2)	27(2)	-4(1)	9(2)	2(1)
C(11)	26(2)	42(2)	28(2)	-3(2)	8(2)	9(2)
C(12)	46(3)	36(2)	37(2)	-8(2)	24(2)	2(2)
C(13)	45(2)	27(2)	31(2)	4(2)	12(2)	4(2)
C(14)	36(2)	30(2)	34(2)	4(2)	5(2)	8(2)
C(15)	30(2)	29(2)	34(2)	-1(1)	13(2)	-2(2)
C(16)	24(2)	33(2)	22(2)	-2(1)	10(2)	3(2)
C(17)	25(2)	36(2)	39(2)	1(2)	8(2)	6(2)
C(18)	45(3)	32(2)	45(2)	-7(2)	20(2)	-4(2)
C(19)	53(3)	26(2)	34(2)	-1(2)	17(2)	8(2)
C(20)	47(3)	38(2)	37(2)	-6(2)	0(2)	19(2)
C(21)	30(2)	34(2)	34(2)	-8(2)	3(2)	7(2)
C(22)	26(2)	23(2)	24(2)	-7(1)	4(2)	-2(1)
C(23)	29(2)	25(2)	41(2)	-2(2)	9(2)	-4(2)
C(24)	37(3)	21(2)	48(2)	1(2)	2(2)	-2(2)
C(25)	35(2)	28(2)	36(2)	-9(2)	-2(2)	9(2)
C(26)	31(2)	52(2)	30(2)	-4(2)	7(2)	12(2)
C(27)	34(2)	40(2)	26(2)	5(2)	6(2)	12(2)
C(28)	28(2)	21(2)	20(2)	4(1)	5(1)	2(1)
C(29)	37(2)	30(2)	32(2)	-4(2)	13(2)	-4(2)
C(30)	51(3)	35(2)	26(2)	-5(2)	13(2)	-2(2)
C(31)	57(3)	28(2)	23(2)	-3(1)	4(2)	-5(2)
C(32)	41(2)	28(2)	41(2)	7(2)	6(2)	-12(2)
C(33)	37(2)	29(2)	27(2)	3(1)	9(2)	0(2)
C(34)	32(2)	20(2)	32(2)	6(1)	11(2)	0(2)
C(35)	74(3)	31(2)	114(4)	-25(2)	70(3)	-19(2)
C(36)	93(4)	31(2)	107(4)	-27(2)	63(3)	-14(2)
C(37)	49(3)	26(2)	42(2)	3(2)	7(2)	-7(2)
C(38)	40(3)	56(2)	37(2)	2(2)	8(2)	-15(2)
C(39)	48(3)	49(2)	29(2)	-10(2)	14(2)	-14(2)
C(40)	35(2)	20(2)	34(2)	1(1)	19(2)	-1(2)
C(41)	37(2)	37(2)	34(2)	6(2)	17(2)	10(2)
C(42)	41(2)	30(2)	44(2)	4(2)	13(2)	11(2)

C(43)	48(3)	36(2)	38(2)	13(2)	10(2)	4(2)
C(44)	55(3)	88(3)	51(3)	34(2)	29(2)	8(2)
C(45)	39(2)	55(2)	44(2)	14(2)	20(2)	2(2)

Table 18. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for (0.84)4 · (0.16)1.

	x	y	z	U(eq)
H(2)	2081	4764	2256	37
H(3)	2523	5024	1685	47
H(4)	2710	3666	988	44
H(5)	2429	2071	838	42
H(6)	1982	1803	1404	36
H(7A)	1968	4143	3442	29
H(7B)	1995	2967	3773	29
H(8A)	1307	3841	1105	33
H(8B)	1377	4573	1955	33
H(9A)	1774	1415	2483	31
H(9B)	1413	1668	1669	31
H(11)	1180	3735	5174	39
H(12)	1354	3347	6691	44
H(13)	1933	2809	7493	42
H(14)	2341	2673	6792	43
H(15)	2174	3099	5275	37
H(17)	1939	5588	4400	41
H(18)	1841	7361	4263	47
H(19)	1262	8004	3556	45
H(20)	784	6864	3103	54
H(21)	884	5075	3272	42
H(23)	808	5279	649	39
H(24)	388	6598	185	47
H(25)	-98	6621	640	45
H(26)	-159	5328	1582	47
H(27)	265	4011	2064	42
H(29)	1055	2625	249	40
H(30)	785	1366	-830	46
H(31)	285	498	-836	47
H(32)	42	885	242	47
H(33)	318	2106	1354	38
H(35)	1317	-162	1756	76
H(36)	950	-1549	1090	84
H(37)	448	-1895	1416	50
H(38)	313	-837	2420	56
H(39)	683	552	3089	50
H(41)	2073	1006	3762	42
H(42)	2453	418	5147	47
H(43)	2239	26	6262	51
H(44)	1637	254	5994	74
H(45)	1254	861	4618	53

Figure 4. Fully-labeled displacement ellipsoid (50%) representation of $[PhB(CH_2PPh_2)_3]Ni(OSiPh_3) \cdot (1.5)C_6H_6$ (**5 · (1.5)C_6H_6**) (hydrogens omitted for clarity).

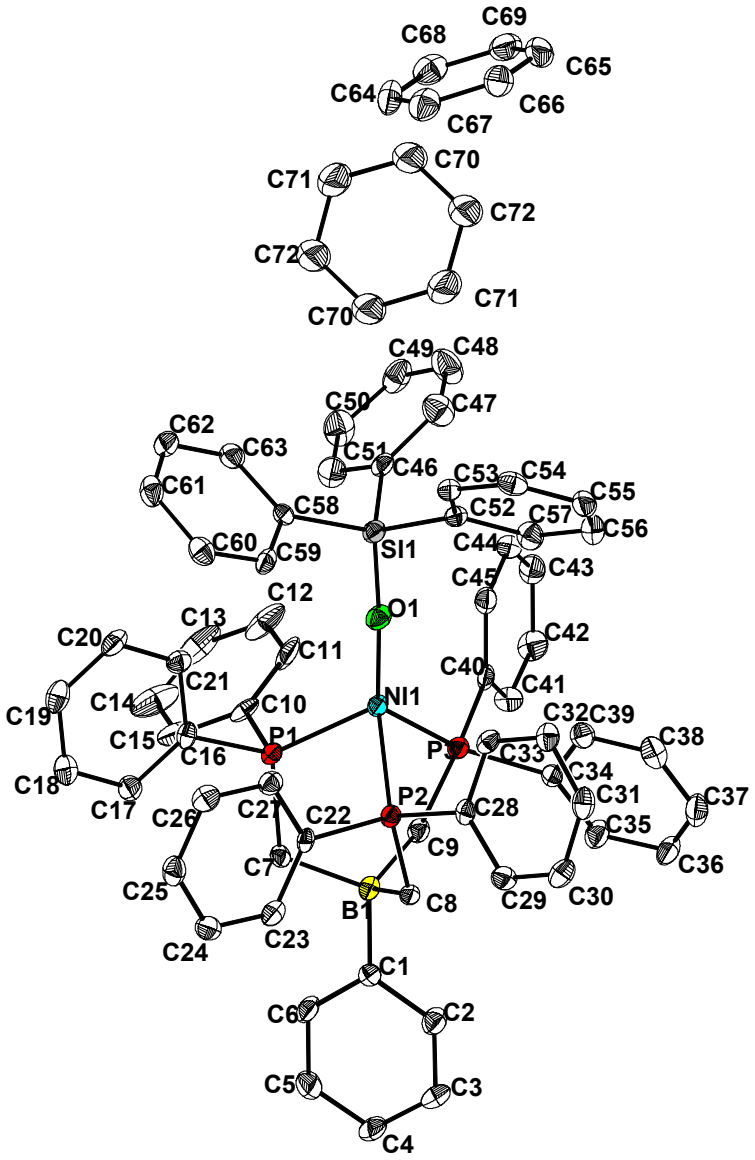


Table 19. Crystal data and structure refinement for 5 · (1.5)C_6H_6.

Empirical formula	$C_{72}H_{65}BNiOP_3Si$	
Moiety formula	$C_{63}H_{56}BNiOP_3Si$, 1.5(C_6H_6)	
Formula weight	1136.76	
Crystal habit	blocks	
Crystal color	green	
Crystal size	0.26 x 0.16 x 0.15 mm^3	
Data Collection		
Type of diffractometer	CCD area detector	
Wavelength	0.71073 Å	
Temperature	96(2) K	
Unit cell dimensions	a = 13.1627(14) Å	α = 101.988(2)°
	b = 14.3575(15) Å	β = 112.185(2)°
	c = 17.2349(18) Å	γ = 90.580(2)°
Volume	2936.1(5) $Å^3$	
Z	2	
Crystal system	Triclinic	
Space group	$P\bar{1}$	
Density (calculated)	1.286 g/cm^3	
F(000)	1194	
θ range for data collection	1.31 to 28.39°	
Completeness to θ = 28.39°	86.0%	
Index ranges	$-17 \le h \le 17$, $-18 \le k \le 17$, $-22 \le l \le 15$	
Reflections collected	18255	
Independent reflections	12668 [R(int) = 0.0568]	
Absorption coefficient	0.478 mm^{-1}	
Absorption correction	None	
Structure solution and refinement		
Structure solution program	SHELXS-97 (Sheldrick, 1990)	
Primary solution method	direct methods	
Secondary solution method	difference Fourier map	
Hydrogen placement	calculated positions	
Structure refinement program	SHELXL-97 (Sheldrick, 1997)	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	12668 / 0 / 712	
Goodness-of-fit on F^2	1.079	
Final R indices [$I>2\sigma(I)$]	R1 = 0.0556, wR2 = 0.0823	
R indices (all data)	R1 = 0.1063, wR2 = 0.0911	
Type of weighting scheme used	calc	
Weighting scheme used	calc $w=1/[\sigma^2(F_o^2)]$	
Max shift/error	0.006	
Average shift/error	0.000	
Largest diff. peak and hole	0.715 and -0.736 $e \cdot Å^{-3}$	

Table 20. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$ x 10^3) for 5 · (1.5)C_6H_6. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
Ni	8700(1)	7158(1)	7370(1)	15(1)
P(1)	10420(1)	6725(1)	7556(1)	15(1)
P(2)	9278(1)	8683(1)	7451(1)	15(1)
P(3)	8079(1)	6799(1)	5905(1)	16(1)
O	8003(2)	6989(2)	8070(1)	22(1)
Si	7409(1)	6609(1)	8622(1)	17(1)
B	10200(3)	7766(3)	6208(2)	16(1)
C(1)	10853(3)	8105(2)	5653(2)	15(1)
C(2)	10370(3)	8676(2)	5070(2)	23(1)
C(3)	10918(3)	9037(2)	4633(2)	28(1)
C(4)	11970(3)	8816(2)	4740(2)	26(1)
C(5)	12458(3)	8230(3)	5277(2)	31(1)
C(6)	11903(3)	7883(2)	5726(2)	24(1)
C(7)	11070(3)	7370(2)	7027(2)	15(1)
C(8)	9663(3)	8737(2)	6561(2)	15(1)
C(9)	9212(3)	6895(2)	5567(2)	17(1)
C(10)	10522(3)	5455(2)	7179(2)	19(1)
C(11)	9603(3)	4802(3)	6772(2)	33(1)
C(12)	9716(4)	3819(3)	6476(2)	47(1)
C(13)	10744(4)	3526(3)	6629(3)	44(1)
C(14)	11660(4)	4163(3)	7046(3)	46(1)
C(15)	11565(3)	5126(2)	7317(2)	33(1)
C(16)	11298(3)	6915(2)	8693(2)	16(1)
C(17)	12374(3)	7315(2)	9055(2)	23(1)
C(18)	13005(3)	7418(2)	9923(2)	27(1)
C(19)	12551(3)	7123(2)	10454(2)	26(1)
C(20)	11469(3)	6722(2)	10103(2)	23(1)
C(21)	10838(3)	6627(2)	9232(2)	19(1)
C(22)	10471(3)	9178(2)	8437(2)	14(1)
C(23)	11404(3)	9665(2)	8451(2)	20(1)
C(24)	12284(3)	10023(2)	9217(2)	22(1)
C(25)	12260(3)	9895(2)	9983(2)	22(1)
C(26)	11338(3)	9422(2)	9982(2)	21(1)
C(27)	10457(3)	9062(2)	9219(2)	19(1)
C(28)	8257(3)	9522(2)	7478(2)	15(1)
C(29)	8233(3)	10367(2)	7181(2)	20(1)
C(30)	7434(3)	10973(2)	7180(2)	24(1)
C(31)	6631(3)	10756(2)	7468(2)	23(1)
C(32)	6619(3)	9928(2)	7754(2)	20(1)
C(33)	7437(3)	9318(2)	7766(2)	17(1)
C(34)	7080(3)	7596(2)	5412(2)	16(1)
C(35)	6970(3)	7862(2)	4647(2)	24(1)
C(36)	6176(3)	8447(2)	4301(2)	30(1)
C(37)	5479(3)	8785(2)	4699(2)	29(1)
C(38)	5569(3)	8532(2)	5447(2)	26(1)
C(39)	6358(3)	7940(2)	5796(2)	20(1)
C(40)	7286(3)	5636(2)	5354(2)	16(1)
C(41)	7224(3)	5173(2)	4546(2)	22(1)
C(42)	6580(3)	4312(2)	4118(2)	27(1)
C(43)	6017(3)	3896(2)	4518(2)	27(1)
C(44)	6079(3)	4349(3)	5325(2)	28(1)
C(45)	6713(3)	5210(2)	5745(2)	20(1)
C(46)	6892(3)	5319(2)	8114(2)	19(1)

C(47)	5802(3)	4955(3)	7805(2)	32(1)
C(48)	5436(3)	4011(3)	7357(3)	37(1)
C(49)	6181(3)	3397(3)	7228(2)	30(1)
C(50)	7278(3)	3728(3)	7557(2)	34(1)
C(51)	7629(3)	4670(2)	7985(2)	28(1)
C(52)	6219(3)	7335(2)	8592(2)	18(1)
C(53)	6047(3)	7830(2)	9318(2)	19(1)
C(54)	5175(3)	8393(2)	9249(2)	22(1)
C(55)	4447(3)	8481(2)	8449(2)	24(1)
C(56)	4589(3)	8000(2)	7722(2)	26(1)
C(57)	5457(3)	7441(2)	7793(2)	23(1)
C(58)	8370(3)	6767(2)	9774(2)	17(1)
C(59)	8875(3)	7684(2)	10250(2)	19(1)
C(60)	9562(3)	7865(2)	11106(2)	24(1)
C(61)	9767(3)	7121(3)	11538(2)	25(1)
C(62)	9295(3)	6206(3)	11093(2)	26(1)
C(63)	8601(3)	6041(2)	10219(2)	21(1)
C(64)	4258(3)	1187(3)	8135(2)	30(1)
C(65)	2052(3)	1388(3)	7319(3)	36(1)
C(66)	2714(3)	2089(3)	8011(3)	33(1)
C(67)	3816(3)	2003(3)	8414(2)	32(1)
C(68)	3603(3)	493(3)	7444(2)	32(1)
C(69)	2498(3)	589(3)	7029(2)	33(1)
C(70)	5800(4)	5594(3)	9963(3)	48(1)
C(71)	4688(4)	5677(3)	9528(3)	47(1)
C(72)	3883(4)	5075(3)	9555(3)	45(1)

Table 21. Selected bond lengths [Å] and angles [°] for 5 · (1.5)C_6H_6.

Ni-O	1.820(2)	O-Ni-P(2)	117.04(7)
Ni-P(2)	2.2695(10)	O-Ni-P(1)	123.59(8)
Ni-P(1)	2.2748(10)	P(2)-Ni-P(1)	89.77(3)
Ni-P(3)	2.2811(10)	O-Ni-P(3)	130.20(8)
Ni-B	3.513(4)	P(2)-Ni-P(3)	91.65(3)
		P(1)-Ni-P(3)	94.06(3)
		Si-O-Ni	168.08(14)

Table 22. Bond lengths [Å] and angles [°] for 5 · (1.5)C_6H_6.

Ni-O	1.820(2)	C(19)-C(20)	1.384(5)
Ni-P(2)	2.2695(10)	C(19)-H(19)	0.9500
Ni-P(1)	2.2748(10)	C(20)-C(21)	1.390(4)
Ni-P(3)	2.2811(10)	C(20)-H(20)	0.9500
Ni-B	3.513(4)	C(21)-H(21)	0.9500
P(1)-C(16)	1.820(3)	C(22)-C(23)	1.398(4)
P(1)-C(10)	1.829(3)	C(22)-C(27)	1.398(4)
P(1)-C(7)	1.829(3)	C(23)-C(24)	1.379(5)
P(2)-C(8)	1.804(3)	C(23)-H(23)	0.9500
P(2)-C(22)	1.822(3)	C(24)-C(25)	1.382(4)
P(2)-C(28)	1.822(3)	C(24)-H(24)	0.9500
P(3)-C(9)	1.806(3)	C(25)-C(26)	1.384(4)
P(3)-C(40)	1.827(3)	C(25)-H(25)	0.9500
P(3)-C(34)	1.830(3)	C(26)-C(27)	1.377(5)
O-Si	1.607(2)	C(26)-H(26)	0.9500
Si-C(58)	1.872(4)	C(27)-H(27)	0.9500
Si-C(46)	1.874(3)	C(28)-C(33)	1.398(4)
Si-C(52)	1.881(3)	C(28)-C(29)	1.407(4)
B-C(1)	1.643(5)	C(29)-C(30)	1.372(4)
B-C(7)	1.659(5)	C(29)-H(29)	0.9500
B-C(9)	1.669(5)	C(30)-C(31)	1.384(4)
B-C(8)	1.674(4)	C(30)-H(30)	0.9500
C(1)-C(6)	1.386(4)	C(31)-C(32)	1.380(4)
C(1)-C(2)	1.398(4)	C(31)-H(31)	0.9500
C(2)-C(3)	1.386(4)	C(32)-C(33)	1.392(4)
C(2)-H(2)	0.9500	C(32)-H(32)	0.9500
C(3)-C(4)	1.375(4)	C(33)-H(33)	0.9500
C(3)-H(3)	0.9500	C(34)-C(39)	1.391(4)
C(4)-C(5)	1.365(4)	C(34)-C(35)	1.404(4)
C(4)-H(4)	0.9500	C(35)-C(36)	1.381(4)
C(5)-C(6)	1.400(4)	C(35)-H(35)	0.9500
C(5)-H(5)	0.9500	C(36)-C(37)	1.376(4)
C(6)-H(6)	0.9500	C(36)-H(36)	0.9500
C(7)-H(7A)	0.9900	C(37)-C(38)	1.374(5)
C(7)-H(7B)	0.9900	C(37)-H(37)	0.9500
C(8)-H(8A)	0.9900	C(38)-C(39)	1.385(4)
C(8)-H(8B)	0.9900	C(38)-H(38)	0.9500
C(9)-H(9A)	0.9900	C(39)-H(39)	0.9500
C(9)-H(9B)	0.9900	C(40)-C(41)	1.383(4)
C(10)-C(11)	1.377(5)	C(40)-C(45)	1.394(4)
C(10)-C(15)	1.406(5)	C(41)-C(42)	1.385(4)
C(11)-C(12)	1.428(5)	C(41)-H(41)	0.9500
C(11)-H(11)	0.9500	C(42)-C(43)	1.388(4)
C(12)-C(13)	1.366(5)	C(42)-H(42)	0.9500
C(12)-H(12)	0.9500	C(43)-C(44)	1.379(4)
C(13)-C(14)	1.363(6)	C(43)-H(43)	0.9500
C(13)-H(13)	0.9500	C(44)-C(45)	1.378(4)
C(14)-C(15)	1.387(5)	C(44)-H(44)	0.9500
C(14)-H(14)	0.9500	C(45)-H(45)	0.9500
C(15)-H(15)	0.9500	C(46)-C(47)	1.380(5)
C(16)-C(17)	1.376(4)	C(46)-C(51)	1.398(4)
C(16)-C(21)	1.407(4)	C(47)-C(48)	1.392(5)
C(17)-C(18)	1.384(4)	C(47)-H(47)	0.9500
C(17)-H(17)	0.9500	C(48)-C(49)	1.374(5)
C(18)-C(19)	1.394(4)	C(48)-H(48)	0.9500
C(18)-H(18)	0.9500	C(49)-C(50)	1.374(5)

C(49)-H(49)	0.9500
C(50)-C(51)	1.380(5)
C(50)-H(50)	0.9500
C(51)-H(51)	0.9500
C(52)-C(53)	1.404(4)
C(52)-C(57)	1.405(5)
C(53)-C(54)	1.393(4)
C(53)-H(53)	0.9500
C(54)-C(55)	1.383(5)
C(54)-H(54)	0.9500
C(55)-C(56)	1.379(4)
C(55)-H(55)	0.9500
C(56)-C(57)	1.385(4)
C(56)-H(56)	0.9500
C(57)-H(57)	0.9500
C(58)-C(63)	1.390(4)
C(58)-C(59)	1.403(4)
C(59)-C(60)	1.374(4)
C(59)-H(59)	0.9500
C(60)-C(61)	1.397(4)
C(60)-H(60)	0.9500
C(61)-C(62)	1.380(5)
C(61)-H(61)	0.9500
C(62)-C(63)	1.402(5)
C(62)-H(62)	0.9500
C(63)-H(63)	0.9500
C(64)-C(68)	1.368(5)
C(64)-C(67)	1.391(5)
C(64)-H(64)	0.9500
C(65)-C(66)	1.376(5)
C(65)-C(69)	1.381(5)
C(65)-H(65)	0.9500
C(66)-C(67)	1.371(5)
C(66)-H(66)	0.9500
C(67)-H(67)	0.9500
C(68)-C(69)	1.381(5)
C(68)-H(68)	0.9500
C(69)-H(69)	0.9500
C(70)-C(72)#1	1.365(5)
C(70)-C(71)	1.389(5)
C(70)-H(70)	0.9500
C(71)-C(72)	1.381(5)
C(71)-H(71)	0.9500
C(72)-C(70)#1	1.365(5)
C(72)-H(72)	0.9500

O-Ni-P(2)	117.04(7)
O-Ni-P(1)	123.59(8)
P(2)-Ni-P(1)	89.77(3)
O-Ni-P(3)	130.20(8)
P(2)-Ni-P(3)	91.65(3)
P(1)-Ni-P(3)	94.06(3)
O-Ni-B	172.60(10)
P(2)-Ni-B	56.18(6)
P(1)-Ni-B	56.32(7)
P(3)-Ni-B	55.68(7)
C(16)-P(1)-C(10)	100.92(15)
C(16)-P(1)-C(7)	109.64(15)
C(10)-P(1)-C(7)	106.20(14)
C(16)-P(1)-Ni	111.16(10)
C(10)-P(1)-Ni	116.37(12)
C(7)-P(1)-Ni	111.87(10)
C(8)-P(2)-C(22)	107.34(15)
C(8)-P(2)-C(28)	108.97(14)
C(22)-P(2)-C(28)	103.62(14)
C(8)-P(2)-Ni	110.57(10)
C(22)-P(2)-Ni	112.51(10)
C(28)-P(2)-Ni	113.45(11)
C(9)-P(3)-C(40)	109.03(14)
C(9)-P(3)-C(34)	107.13(14)
C(40)-P(3)-C(34)	100.66(15)
C(9)-P(3)-Ni	110.44(11)
C(40)-P(3)-Ni	115.98(11)
C(34)-P(3)-Ni	112.91(11)
Si-O-Ni	168.08(14)
O-Si-C(58)	111.39(14)
O-Si-C(46)	108.27(13)
C(58)-Si-C(46)	111.11(15)
O-Si-C(52)	108.15(13)
C(58)-Si-C(52)	107.95(14)
C(46)-Si-C(52)	109.93(15)
C(1)-B-C(7)	110.2(3)
C(1)-B-C(9)	109.2(3)
C(7)-B-C(9)	109.5(3)
C(1)-B-C(8)	105.9(3)
C(7)-B-C(8)	110.8(3)
C(9)-B-C(8)	111.1(3)
C(1)-B-Ni	176.4(2)
C(7)-B-Ni	72.67(16)
C(9)-B-Ni	71.18(16)
C(8)-B-Ni	70.82(15)
C(6)-C(1)-C(2)	114.8(3)
C(6)-C(1)-B	124.5(3)
C(2)-C(1)-B	120.7(3)
C(3)-C(2)-C(1)	122.8(3)
C(3)-C(2)-H(2)	118.6
C(1)-C(2)-H(2)	118.6
C(4)-C(3)-C(2)	120.3(3)
C(4)-C(3)-H(3)	119.8
C(2)-C(3)-H(3)	119.8
C(5)-C(4)-C(3)	118.9(3)
C(5)-C(4)-H(4)	120.6
C(3)-C(4)-H(4)	120.6
C(4)-C(5)-C(6)	120.2(3)
C(4)-C(5)-H(5)	119.9
C(6)-C(5)-H(5)	119.9
C(1)-C(6)-C(5)	122.9(3)
C(1)-C(6)-H(6)	118.5
C(5)-C(6)-H(6)	118.5
B-C(7)-P(1)	114.9(2)
B-C(7)-H(7A)	108.5
P(1)-C(7)-H(7A)	108.5
B-C(7)-H(7B)	108.5
P(1)-C(7)-H(7B)	108.5
H(7A)-C(7)-H(7B)	107.5
B-C(8)-P(2)	115.1(2)

B-C(8)-H(8A)	108.5	C(26)-C(25)-H(25)	120.1
P(2)-C(8)-H(8A)	108.5	C(27)-C(26)-C(25)	120.1(3)
B-C(8)-H(8B)	108.5	C(27)-C(26)-H(26)	119.9
P(2)-C(8)-H(8B)	108.5	C(25)-C(26)-H(26)	119.9
H(8A)-C(8)-H(8B)	107.5	C(26)-C(27)-C(22)	120.9(3)
B-C(9)-P(3)	114.1(2)	C(26)-C(27)-H(27)	119.6
B-C(9)-H(9A)	108.7	C(22)-C(27)-H(27)	119.6
P(3)-C(9)-H(9A)	108.7	C(33)-C(28)-C(29)	118.0(3)
B-C(9)-H(9B)	108.7	C(33)-C(28)-P(2)	120.1(2)
P(3)-C(9)-H(9B)	108.7	C(29)-C(28)-P(2)	121.9(2)
H(9A)-C(9)-H(9B)	107.6	C(30)-C(29)-C(28)	120.9(3)
C(11)-C(10)-C(15)	118.7(3)	C(30)-C(29)-H(29)	119.5
C(11)-C(10)-P(1)	121.8(3)	C(28)-C(29)-H(29)	119.5
C(15)-C(10)-P(1)	119.5(3)	C(29)-C(30)-C(31)	120.1(3)
C(10)-C(11)-C(12)	120.1(4)	C(29)-C(30)-H(30)	119.9
C(10)-C(11)-H(11)	120.0	C(31)-C(30)-H(30)	119.9
C(12)-C(11)-H(11)	120.0	C(32)-C(31)-C(30)	120.6(3)
C(13)-C(12)-C(11)	119.5(4)	C(32)-C(31)-H(31)	119.7
C(13)-C(12)-H(12)	120.2	C(30)-C(31)-H(31)	119.7
C(11)-C(12)-H(12)	120.2	C(31)-C(32)-C(33)	119.4(3)
C(14)-C(13)-C(12)	120.8(4)	C(31)-C(32)-H(32)	120.3
C(14)-C(13)-H(13)	119.6	C(33)-C(32)-H(32)	120.3
C(12)-C(13)-H(13)	119.6	C(32)-C(33)-C(28)	121.0(3)
C(13)-C(14)-C(15)	120.5(4)	C(32)-C(33)-H(33)	119.5
C(13)-C(14)-H(14)	119.7	C(28)-C(33)-H(33)	119.5
C(15)-C(14)-H(14)	119.7	C(39)-C(34)-C(35)	117.3(3)
C(14)-C(15)-C(10)	120.4(4)	C(39)-C(34)-P(3)	118.8(2)
C(14)-C(15)-H(15)	119.8	C(35)-C(34)-P(3)	123.9(2)
C(10)-C(15)-H(15)	119.8	C(36)-C(35)-C(34)	120.6(3)
C(17)-C(16)-C(21)	118.3(3)	C(36)-C(35)-H(35)	119.7
C(17)-C(16)-P(1)	124.4(3)	C(34)-C(35)-H(35)	119.7
C(21)-C(16)-P(1)	117.3(3)	C(37)-C(36)-C(35)	120.8(3)
C(16)-C(17)-C(18)	121.4(3)	C(37)-C(36)-H(36)	119.6
C(16)-C(17)-H(17)	119.3	C(35)-C(36)-H(36)	119.6
C(18)-C(17)-H(17)	119.3	C(38)-C(37)-C(36)	119.6(3)
C(17)-C(18)-C(19)	120.2(4)	C(38)-C(37)-H(37)	120.2
C(17)-C(18)-H(18)	119.9	C(36)-C(37)-H(37)	120.2
C(19)-C(18)-H(18)	119.9	C(37)-C(38)-C(39)	120.0(3)
C(20)-C(19)-C(18)	119.3(3)	C(37)-C(38)-H(38)	120.0
C(20)-C(19)-H(19)	120.3	C(39)-C(38)-H(38)	120.0
C(18)-C(19)-H(19)	120.3	C(38)-C(39)-C(34)	121.7(3)
C(19)-C(20)-C(21)	120.2(3)	C(38)-C(39)-H(39)	119.2
C(19)-C(20)-H(20)	119.9	C(34)-C(39)-H(39)	119.2
C(21)-C(20)-H(20)	119.9	C(41)-C(40)-C(45)	119.0(3)
C(20)-C(21)-C(16)	120.6(3)	C(41)-C(40)-P(3)	121.4(2)
C(20)-C(21)-H(21)	119.7	C(45)-C(40)-P(3)	119.6(2)
C(16)-C(21)-H(21)	119.7	C(40)-C(41)-C(42)	120.9(3)
C(23)-C(22)-C(27)	118.3(3)	C(40)-C(41)-H(41)	119.6
C(23)-C(22)-P(2)	123.1(2)	C(42)-C(41)-H(41)	119.6
C(27)-C(22)-P(2)	118.6(2)	C(41)-C(42)-C(43)	119.3(3)
C(24)-C(23)-C(22)	120.6(3)	C(41)-C(42)-H(42)	120.3
C(24)-C(23)-H(23)	119.7	C(43)-C(42)-H(42)	120.3
C(22)-C(23)-H(23)	119.7	C(44)-C(43)-C(42)	120.2(3)
C(23)-C(24)-C(25)	120.4(3)	C(44)-C(43)-H(43)	119.9
C(23)-C(24)-H(24)	119.8	C(42)-C(43)-H(43)	119.9
C(25)-C(24)-H(24)	119.8	C(45)-C(44)-C(43)	120.2(3)
C(24)-C(25)-C(26)	119.8(3)	C(45)-C(44)-H(44)	119.9
C(24)-C(25)-H(25)	120.1	C(43)-C(44)-H(44)	119.9

C(44)-C(45)-C(40)	120.4(3)	C(60)-C(59)-C(58)	122.7(3)
C(44)-C(45)-H(45)	119.8	C(60)-C(59)-H(59)	118.6
C(40)-C(45)-H(45)	119.8	C(58)-C(59)-H(59)	118.6
C(47)-C(46)-C(51)	116.1(3)	C(59)-C(60)-C(61)	119.8(3)
C(47)-C(46)-Si	124.6(3)	C(59)-C(60)-H(60)	120.1
C(51)-C(46)-Si	119.2(3)	C(61)-C(60)-H(60)	120.1
C(46)-C(47)-C(48)	122.8(3)	C(62)-C(61)-C(60)	119.5(3)
C(46)-C(47)-H(47)	118.6	C(62)-C(61)-H(61)	120.3
C(48)-C(47)-H(47)	118.6	C(60)-C(61)-H(61)	120.3
C(49)-C(48)-C(47)	119.6(4)	C(61)-C(62)-C(63)	119.5(3)
C(49)-C(48)-H(48)	120.2	C(61)-C(62)-H(62)	120.2
C(47)-C(48)-H(48)	120.2	C(63)-C(62)-H(62)	120.3
C(48)-C(49)-C(50)	119.0(4)	C(58)-C(63)-C(62)	122.4(3)
C(48)-C(49)-H(49)	120.5	C(58)-C(63)-H(63)	118.8
C(50)-C(49)-H(49)	120.5	C(62)-C(63)-H(63)	118.8
C(49)-C(50)-C(51)	120.9(3)	C(68)-C(64)-C(67)	120.0(4)
C(49)-C(50)-H(50)	119.6	C(68)-C(64)-H(64)	120.0
C(51)-C(50)-H(50)	119.6	C(67)-C(64)-H(64)	120.0
C(50)-C(51)-C(46)	121.6(3)	C(66)-C(65)-C(69)	119.9(4)
C(50)-C(51)-H(51)	119.2	C(66)-C(65)-H(65)	120.0
C(46)-C(51)-H(51)	119.2	C(69)-C(65)-H(65)	120.0
C(53)-C(52)-C(57)	115.9(3)	C(67)-C(66)-C(65)	120.5(4)
C(53)-C(52)-Si	125.1(3)	C(67)-C(66)-H(66)	119.8
C(57)-C(52)-Si	119.0(3)	C(65)-C(66)-H(66)	119.8
C(54)-C(53)-C(52)	122.0(3)	C(66)-C(67)-C(64)	119.6(4)
C(54)-C(53)-H(53)	119.0	C(66)-C(67)-H(67)	120.2
C(52)-C(53)-H(53)	119.0	C(64)-C(67)-H(67)	120.2
C(55)-C(54)-C(53)	120.2(3)	C(64)-C(68)-C(69)	120.4(4)
C(55)-C(54)-H(54)	119.9	C(64)-C(68)-H(68)	119.8
C(53)-C(54)-H(54)	119.9	C(69)-C(68)-H(68)	119.8
C(56)-C(55)-C(54)	119.3(3)	C(65)-C(69)-C(68)	119.7(4)
C(56)-C(55)-H(55)	120.3	C(65)-C(69)-H(69)	120.2
C(54)-C(55)-H(55)	120.3	C(68)-C(69)-H(69)	120.2
C(55)-C(56)-C(57)	120.3(3)	C(72)#1-C(70)-C(71)	120.3(4)
C(55)-C(56)-H(56)	119.8	C(72)#1-C(70)-H(70)	119.8
C(57)-C(56)-H(56)	119.8	C(71)-C(70)-H(70)	119.8
C(56)-C(57)-C(52)	122.3(3)	C(72)-C(71)-C(70)	121.1(4)
C(56)-C(57)-H(57)	118.9	C(72)-C(71)-H(71)	119.5
C(52)-C(57)-H(57)	118.9	C(70)-C(71)-H(71)	119.5
C(63)-C(58)-C(59)	116.0(3)	C(70)#1-C(72)-C(71)	118.6(4)
C(63)-C(58)-Si	124.8(3)	C(70)#1-C(72)-H(72)	120.7
C(59)-C(58)-Si	119.2(2)	C(71)-C(72)-H(72)	120.7

Symmetry transformations used to generate equivalent atoms:
#1 -x+1,-y+1,-z+2

Table 23. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for 5 · (1.5)C_6H_6. The anisotropic displacement factor exponent takes the form: $-2\pi^2[\ h^2 a^{*2} U^{11} + ... + 2\ h\ k\ a^*\ b^*\ U^{12}]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Ni	16(1)	15(1)	14(1)	5(1)	4(1)	1(1)
P(1)	17(1)	13(1)	13(1)	4(1)	5(1)	2(1)
P(2)	15(1)	13(1)	15(1)	4(1)	4(1)	2(1)
P(3)	16(1)	16(1)	14(1)	4(1)	4(1)	1(1)
O	25(1)	26(1)	21(1)	10(1)	13(1)	8(1)
Si	19(1)	18(1)	16(1)	6(1)	7(1)	2(1)
B	17(2)	18(2)	14(2)	5(2)	6(2)	4(2)
C(1)	17(2)	13(2)	14(2)	1(2)	5(2)	0(2)
C(2)	23(2)	30(2)	21(2)	11(2)	11(2)	9(2)
C(3)	32(2)	33(2)	27(2)	19(2)	12(2)	3(2)
C(4)	29(2)	35(2)	22(2)	16(2)	14(2)	5(2)
C(5)	18(2)	48(3)	33(2)	18(2)	13(2)	7(2)
C(6)	24(2)	34(2)	21(2)	18(2)	11(2)	12(2)
C(7)	12(2)	20(2)	15(2)	5(2)	7(2)	4(2)
C(8)	14(2)	14(2)	15(2)	5(2)	3(2)	-1(1)
C(9)	18(2)	20(2)	13(2)	5(2)	5(2)	3(2)
C(10)	35(2)	14(2)	10(2)	5(2)	10(2)	3(2)
C(11)	39(3)	28(2)	19(2)	15(2)	-7(2)	-1(2)
C(12)	82(4)	22(2)	14(2)	6(2)	-7(2)	-15(2)
C(13)	93(4)	22(2)	25(3)	9(2)	29(3)	21(3)
C(14)	86(4)	33(3)	55(3)	23(2)	58(3)	28(3)
C(15)	52(3)	21(2)	44(3)	16(2)	35(2)	11(2)
C(16)	18(2)	14(2)	13(2)	2(2)	4(2)	6(2)
C(17)	18(2)	33(2)	18(2)	10(2)	7(2)	3(2)
C(18)	21(2)	33(2)	23(2)	9(2)	1(2)	1(2)
C(19)	29(2)	32(2)	13(2)	6(2)	2(2)	6(2)
C(20)	29(2)	25(2)	20(2)	13(2)	11(2)	9(2)
C(21)	21(2)	15(2)	21(2)	6(2)	7(2)	1(2)
C(22)	14(2)	11(2)	15(2)	4(2)	3(2)	6(1)
C(23)	23(2)	21(2)	18(2)	9(2)	8(2)	6(2)
C(24)	20(2)	23(2)	21(2)	5(2)	8(2)	-1(2)
C(25)	21(2)	21(2)	17(2)	2(2)	1(2)	1(2)
C(26)	27(2)	22(2)	15(2)	3(2)	9(2)	2(2)
C(27)	20(2)	19(2)	20(2)	7(2)	10(2)	5(2)
C(28)	16(2)	13(2)	10(2)	-1(1)	0(2)	0(1)
C(29)	19(2)	20(2)	21(2)	5(2)	7(2)	-1(2)
C(30)	30(2)	18(2)	26(2)	9(2)	10(2)	8(2)
C(31)	22(2)	21(2)	22(2)	3(2)	6(2)	10(2)
C(32)	19(2)	24(2)	14(2)	2(2)	6(2)	6(2)
C(33)	22(2)	14(2)	10(2)	2(2)	2(2)	-1(2)
C(34)	15(2)	12(2)	16(2)	3(2)	0(2)	-4(1)
C(35)	25(2)	29(2)	17(2)	9(2)	6(2)	5(2)
C(36)	28(2)	31(2)	28(2)	18(2)	1(2)	2(2)
C(37)	22(2)	22(2)	31(2)	9(2)	-2(2)	3(2)
C(38)	20(2)	25(2)	28(2)	1(2)	6(2)	2(2)
C(39)	20(2)	20(2)	17(2)	2(2)	4(2)	-1(2)
C(40)	14(2)	17(2)	16(2)	7(2)	2(2)	5(2)
C(41)	25(2)	21(2)	23(2)	5(2)	11(2)	0(2)
C(42)	32(2)	27(2)	17(2)	1(2)	7(2)	-1(2)
C(43)	24(2)	17(2)	28(2)	4(2)	0(2)	-3(2)
C(44)	20(2)	31(2)	32(2)	17(2)	4(2)	-4(2)
C(45)	18(2)	19(2)	18(2)	5(2)	2(2)	2(2)
C(46)	21(2)	23(2)	14(2)	9(2)	7(2)	4(2)

C(47)	28(2)	29(2)	39(3)	4(2)	15(2)	5(2)
C(48)	25(2)	25(2)	50(3)	2(2)	5(2)	-4(2)
C(49)	39(3)	19(2)	24(2)	5(2)	2(2)	2(2)
C(50)	34(3)	23(2)	40(3)	4(2)	10(2)	8(2)
C(51)	28(2)	21(2)	28(2)	3(2)	6(2)	1(2)
C(52)	18(2)	17(2)	17(2)	7(2)	4(2)	-2(2)
C(53)	17(2)	18(2)	22(2)	8(2)	5(2)	-1(2)
C(54)	23(2)	20(2)	27(2)	2(2)	16(2)	1(2)
C(55)	17(2)	22(2)	32(2)	10(2)	7(2)	3(2)
C(56)	20(2)	31(2)	27(2)	10(2)	6(2)	6(2)
C(57)	23(2)	25(2)	18(2)	2(2)	6(2)	0(2)
C(58)	11(2)	23(2)	21(2)	10(2)	9(2)	4(2)
C(59)	20(2)	19(2)	19(2)	10(2)	6(2)	7(2)
C(60)	20(2)	25(2)	21(2)	1(2)	6(2)	-1(2)
C(61)	19(2)	40(2)	14(2)	6(2)	5(2)	6(2)
C(62)	22(2)	37(2)	23(2)	16(2)	9(2)	5(2)
C(63)	18(2)	22(2)	25(2)	6(2)	9(2)	3(2)
C(64)	27(2)	45(3)	24(2)	14(2)	12(2)	16(2)
C(65)	22(2)	32(2)	56(3)	21(2)	11(2)	6(2)
C(66)	28(3)	29(2)	48(3)	17(2)	17(2)	12(2)
C(67)	36(3)	40(2)	28(2)	11(2)	17(2)	10(2)
C(68)	41(3)	32(2)	34(3)	13(2)	23(2)	12(2)
C(69)	37(3)	28(2)	31(2)	12(2)	9(2)	-4(2)
C(70)	33(3)	52(3)	75(4)	37(3)	26(3)	12(2)
C(71)	41(3)	49(3)	64(3)	34(3)	24(3)	17(2)
C(72)	33(3)	43(3)	67(3)	28(3)	20(2)	8(2)

Table 24. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for 5 · (1.5)C_6H_6.

	x	y	z	U(eq)
H(2)	9635	8822	4969	28
H(3)	10566	9440	4257	34
H(4)	12350	9066	4445	31
H(5)	13177	8057	5347	37
H(6)	12261	7477	6096	28
H(7A)	11557	7923	7460	18
H(7B)	11541	6942	6816	18
H(8A)	9002	8839	6076	18
H(8B)	10207	9299	6736	18
H(9A)	9541	6278	5543	21
H(9B)	8920	7007	4978	21
H(11)	8893	5006	6689	39
H(12)	9082	3372	6174	56
H(13)	10822	2869	6443	53
H(14)	12369	3947	7152	56
H(15)	12208	5566	7598	39
H(17)	12692	7525	8701	27
H(18)	13748	7690	10157	33
H(19)	12980	7197	11050	31
H(20)	11155	6511	10459	27
H(21)	10091	6364	8999	22
H(23)	11432	9751	7927	24
H(24)	12911	10359	9219	26
H(25)	12874	10131	10509	27
H(26)	11312	9346	10510	26
H(27)	9832	8731	9224	22
H(29)	8778	10519	6978	24
H(30)	7433	11543	6982	29
H(31)	6082	11181	7468	27
H(32)	6058	9776	7941	23
H(33)	7439	8754	7973	20
H(35)	7445	7638	4364	29
H(36)	6111	8619	3782	36
H(37)	4938	9190	4458	34
H(38)	5091	8763	5726	31
H(39)	6406	7765	6310	24
H(41)	7628	5449	4282	27
H(42)	6524	4008	3557	32
H(43)	5588	3298	4235	32
H(44)	5684	4066	5592	33
H(45)	6759	5514	6304	23
H(47)	5281	5367	7902	38
H(48)	4676	3793	7142	45
H(49)	5941	2753	6917	37
H(50)	7802	3302	7489	41
H(51)	8391	4884	8198	33
H(53)	6540	7780	9873	23
H(54)	5080	8718	9753	27
H(55)	3854	8868	8400	29
H(56)	4090	8054	7170	31
H(57)	5539	7117	7283	27
H(59)	8737	8201	9970	23
H(60)	9897	8495	11403	28

H(61)	10227	7244	12132	30
H(62)	9440	5692	11377	31
H(63)	8278	5409	9921	25
H(64)	5016	1112	8424	36
H(65)	1290	1453	7041	43
H(66)	2404	2636	8212	39
H(67)	4274	2498	8880	39
H(68)	3910	-59	7248	38
H(69)	2046	108	6546	39
H(70)	6341	6003	9925	58
H(71)	4479	6157	9207	56
H(72)	3124	5125	9244	54

Figure 5. Fully-labeled displacement ellipsoid (50%) representation of [PhB(CH_2PPh_2)$_3$]Ni(S-*p*-^{t}Bu-Ph) (**7**) (hydrogens omitted for clarity).

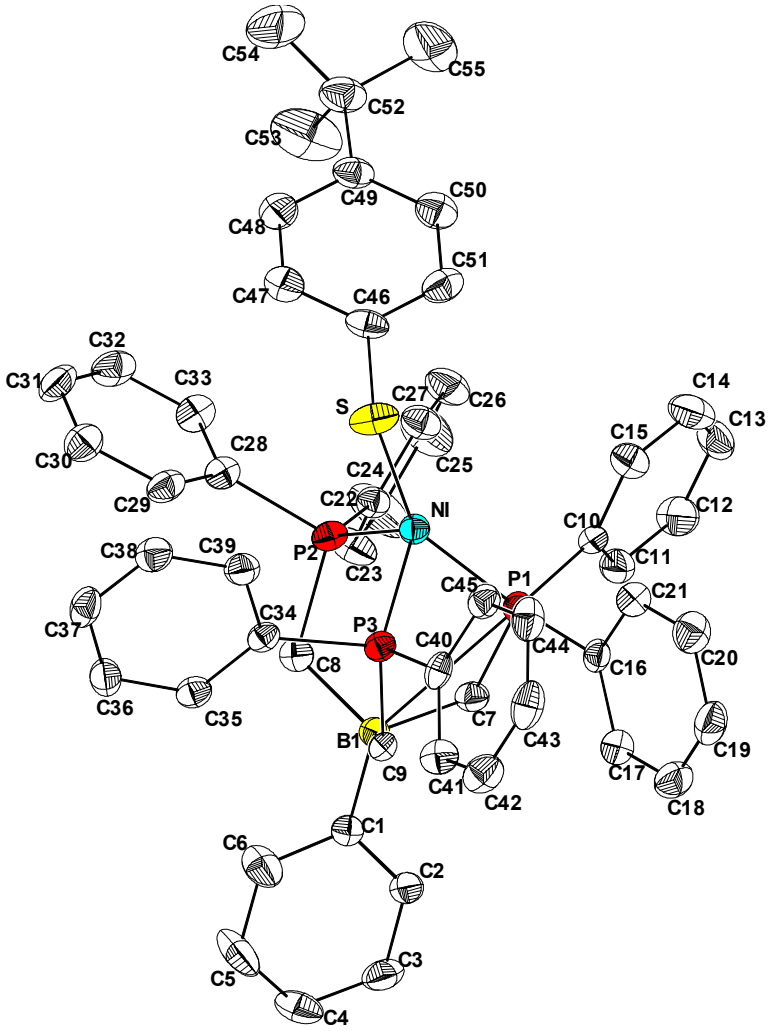


Table 25. Crystal data and structure refinement for 7.

Empirical formula	$C_{55}H_{54}BNiP_3S$	
Moiety formula	$C_{55}H_{54}BNiP_3S$	
Formula weight	909.47	
Crystal habit	prism	
Crystal color	black-purple	
Crystal size	0.13 x 0.33 x 0.41 mm^3	
Data Collection		
Type of diffractometer	CCD area detector	
Wavelength	0.71073 Å	
Temperature	100(2) K	
Unit cell dimensions	a = 38.222(2) Å	α = 90°
	b = 38.222(2) Å	β = 90°
	c = 12.5712(9) Å	γ = 90°
Volume	18366.0(19) $Å^3$	
Z	16	
Crystal system	Tetragonal	
Space group	$I4_1/a$	
Density (calculated)	1.316 g/cm^3	
F(000)	7648	
θ range for data collection	1.51 to 28.67°	
Completeness to θ = 28.67°	93.7%	
Index ranges	$-51 \le h \le 51$, $-49 \le k \le 49$, $-16 \le l \le 16$	
Reflections collected	83862	
Independent reflections	11088 [R(int) = 0.1080]	
Absorption coefficient	0.610 mm^{-1}	
Absorption correction	None	
Structure solution and refinement		
Structure solution program	SHELXS-97 (Sheldrick, 1990)	
Primary solution method	direct methods	
Secondary solution method	difference Fourier map	
Hydrogen placement	calculated positions	
Structure refinement program	SHELXL-97 (Sheldrick, 1997)	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	11088 / 0 / 553	
Goodness-of-fit on F^2	1.388	
Final R indices [$I>2\sigma(I)$]	R1 = 0.0523, wR2 = 0.0648	
R indices (all data)	R1 = 0.1198, wR2 = 0.0706	
Type of weighting scheme used	calculated	
Weighting scheme used	calc $w=1/[\sigma^2(F_o^2)]$	
Max shift/error	0.001	
Average shift/error	0.000	
Largest diff. peak and hole	1.018 and -0.858 $e \cdot Å^{-3}$	

Table 26. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$ x 10^3) for 7. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
Ni	3954(1)	831(1)	1267(1)	21(1)
P(1)	4229(1)	906(1)	2778(1)	23(1)
P(2)	4404(1)	537(1)	666(1)	24(1)
P(3)	3583(1)	449(1)	2019(1)	22(1)
S	3652(1)	1020(1)	-24(1)	36(1)
B(1)	4273(1)	163(1)	2737(2)	21(1)
C(2)	4575(1)	-169(1)	4364(2)	28(1)
C(3)	4658(1)	-469(1)	4940(2)	35(1)
C(4)	4573(1)	-790(1)	4558(2)	37(1)
C(5)	4403(1)	-812(1)	3602(3)	49(1)
C(6)	4323(1)	-513(1)	3031(2)	40(1)
C(1)	4405(1)	-179(1)	3390(2)	21(1)
C(7)	4461(1)	526(1)	3204(2)	24(1)
C(8)	4386(1)	132(1)	1450(2)	23(1)
C(9)	3839(1)	180(1)	2924(2)	22(1)
C(30)	4061(1)	93(1)	-2098(2)	33(1)
C(31)	4327(1)	156(1)	-2819(2)	37(1)
C(32)	4620(1)	335(1)	-2500(2)	37(1)
C(33)	4650(1)	453(1)	-1459(2)	29(1)
C(22)	4843(1)	720(1)	722(2)	23(1)
C(23)	5141(1)	528(1)	955(2)	38(1)
C(24)	5468(1)	676(1)	860(3)	60(1)
C(25)	5503(1)	1017(1)	537(3)	49(1)
C(26)	5213(1)	1212(1)	306(2)	39(1)
C(27)	4886(1)	1065(1)	402(2)	31(1)
C(28)	4384(1)	393(1)	-733(2)	24(1)
C(29)	4087(1)	215(1)	-1066(2)	29(1)
C(10)	4527(1)	1279(1)	2783(2)	23(1)
C(11)	4861(1)	1257(1)	3210(2)	31(1)
C(12)	5077(1)	1548(1)	3252(2)	38(1)
C(13)	4958(1)	1865(1)	2875(2)	39(1)
C(14)	4632(1)	1889(1)	2436(2)	42(1)
C(15)	4419(1)	1598(1)	2375(2)	31(1)
C(16)	3917(1)	1028(1)	3815(2)	22(1)
C(21)	3684(1)	1297(1)	3608(2)	28(1)
C(20)	3431(1)	1395(1)	4349(2)	35(1)
C(19)	3406(1)	1216(1)	5293(2)	37(1)
C(18)	3635(1)	946(1)	5503(2)	37(1)
C(17)	3892(1)	851(1)	4780(2)	29(1)
C(40)	3184(1)	583(1)	2686(2)	22(1)
C(45)	3026(1)	904(1)	2434(2)	26(1)
C(44)	2721(1)	1005(1)	2932(2)	32(1)
C(43)	2568(1)	791(1)	3677(2)	35(1)
C(42)	2716(1)	474(1)	3932(2)	34(1)
C(41)	3024(1)	371(1)	3445(2)	28(1)
C(34)	3409(1)	149(1)	1015(2)	21(1)
C(39)	3182(1)	279(1)	244(2)	28(1)
C(38)	3069(1)	71(1)	-582(2)	30(1)
C(37)	3178(1)	-270(1)	-657(2)	31(1)
C(36)	3391(1)	-410(1)	122(2)	29(1)
C(35)	3506(1)	-202(1)	950(2)	25(1)
C(46)	3947(1)	1228(1)	-907(2)	29(1)
C(51)	4113(1)	1535(1)	-642(2)	34(1)

C(50)	4348(1)	1697(1)	-1342(2)	35(1)
C(49)	4418(1)	1550(1)	-2330(2)	30(1)
C(48)	4243(1)	1245(1)	-2586(2)	37(1)
C(47)	4012(1)	1088(1)	-1908(2)	36(1)
C(52)	4688(1)	1704(1)	-3091(2)	41(1)
C(55)	4786(1)	2076(1)	-2818(3)	64(1)
C(53)	5015(1)	1473(1)	-3022(3)	77(1)
C(54)	4547(1)	1697(1)	-4224(2)	74(1)

Table 27. Selected bond lengths [Å] and angles [°] for 7.

Ni-S	2.1188(8)
Ni-P(2)	2.1878(8)
Ni-P(1)	2.1890(8)
Ni-P(3)	2.2439(8)
Ni-B(1)	3.380(3)
S-Ni-P(2)	109.79(3)
S-Ni-P(1)	151.84(3)
P(2)-Ni-P(1)	89.44(3)
S-Ni-P(3)	101.54(3)
P(2)-Ni-P(3)	107.87(3)
P(1)-Ni-P(3)	91.28(3)

Table 28. Bond lengths [Å] and angles [°] for 7.

Ni-S	2.1188(8)	C(28)-C(29)	1.388(3)
Ni-P(2)	2.1878(8)	C(29)-H(23)	0.9500
Ni-P(1)	2.1890(8)	C(10)-C(15)	1.385(3)
Ni-P(3)	2.2439(8)	C(10)-C(11)	1.387(3)
Ni-B(1)	3.380(3)	C(11)-C(12)	1.388(4)
P(1)-C(7)	1.784(2)	C(11)-H(25)	0.9500
P(1)-C(10)	1.826(3)	C(12)-C(13)	1.379(4)
P(1)-C(16)	1.827(3)	C(12)-H(26)	0.9500
P(2)-C(22)	1.822(3)	C(13)-C(14)	1.366(4)
P(2)-C(8)	1.835(2)	C(13)-H(27)	0.9500
P(2)-C(28)	1.844(3)	C(14)-C(15)	1.381(4)
P(3)-C(40)	1.815(3)	C(14)-H(28)	0.9500
P(3)-C(9)	1.819(2)	C(15)-H(29)	0.9500
P(3)-C(34)	1.832(3)	C(16)-C(21)	1.384(3)
S-C(46)	1.768(3)	C(16)-C(17)	1.393(3)
B(1)-C(1)	1.626(4)	C(21)-C(20)	1.394(3)
B(1)-C(7)	1.667(4)	C(21)-H(31)	0.9500
B(1)-C(8)	1.678(4)	C(20)-C(19)	1.373(4)
B(1)-C(9)	1.680(4)	C(20)-H(32)	0.9500
C(2)-C(1)	1.387(3)	C(19)-C(18)	1.379(4)
C(2)-C(3)	1.393(3)	C(19)-H(33)	0.9500
C(2)-H(1)	0.9500	C(18)-C(17)	1.387(3)
C(3)-C(4)	1.358(4)	C(18)-H(34)	0.9500
C(3)-H(2)	0.9500	C(17)-H(35)	0.9500
C(4)-C(5)	1.369(4)	C(40)-C(41)	1.392(3)
C(4)-H(3)	0.9500	C(40)-C(45)	1.404(3)
C(5)-C(6)	1.384(4)	C(45)-C(44)	1.380(3)
C(5)-H(4)	0.9500	C(45)-H(37)	0.9500
C(6)-C(1)	1.387(3)	C(44)-C(43)	1.376(4)
C(6)-H(5)	0.9500	C(44)-H(38)	0.9500
C(7)-H(7A)	0.9900	C(43)-C(42)	1.373(4)
C(7)-H(7B)	0.9900	C(43)-H(39)	0.9500
C(8)-H(8A)	0.9900	C(42)-C(41)	1.386(3)
C(8)-H(8B)	0.9900	C(42)-H(40)	0.9500
C(9)-H(9A)	0.9900	C(41)-H(41)	0.9500
C(9)-H(9B)	0.9900	C(34)-C(39)	1.393(3)
C(30)-C(29)	1.381(3)	C(34)-C(35)	1.393(3)
C(30)-C(31)	1.383(4)	C(39)-C(38)	1.377(3)
C(30)-H(12)	0.9500	C(39)-H(43)	0.9500
C(31)-C(32)	1.371(4)	C(38)-C(37)	1.372(4)
C(31)-H(13)	0.9500	C(38)-H(44)	0.9500
C(32)-C(33)	1.390(3)	C(37)-C(36)	1.382(3)
C(32)-H(14)	0.9500	C(37)-H(45)	0.9500
C(33)-C(28)	1.385(3)	C(36)-C(35)	1.382(3)
C(33)-H(15)	0.9500	C(36)-H(46)	0.9500
C(22)-C(27)	1.386(3)	C(35)-H(47)	0.9500
C(22)-C(23)	1.388(3)	C(46)-C(51)	1.377(4)
C(23)-C(24)	1.377(4)	C(46)-C(47)	1.390(3)
C(23)-H(17)	0.9500	C(51)-C(50)	1.400(3)
C(24)-C(25)	1.369(4)	C(51)-H(49)	0.9500
C(24)-H(18)	0.9500	C(50)-C(49)	1.388(4)
C(25)-C(26)	1.368(4)	C(50)-H(50)	0.9500
C(25)-H(19)	0.9500	C(49)-C(48)	1.383(4)
C(26)-C(27)	1.377(3)	C(49)-C(52)	1.524(4)
C(26)-H(20)	0.9500	C(48)-C(47)	1.367(4)
C(27)-H(21)	0.9500	C(48)-H(52)	0.9500

C(47)-H(53)	0.9500	C(3)-C(4)-C(5)	118.6(3)
C(52)-C(55)	1.508(4)	C(3)-C(4)-H(3)	120.7
C(52)-C(54)	1.523(4)	C(5)-C(4)-H(3)	120.7
C(52)-C(53)	1.533(4)	C(4)-C(5)-C(6)	120.6(3)
C(55)-H(55A)	0.9800	C(4)-C(5)-H(4)	119.7
C(55)-H(55B)	0.9800	C(6)-C(5)-H(4)	119.7
C(55)-H(55C)	0.9800	C(5)-C(6)-C(1)	122.7(3)
C(53)-H(56A)	0.9800	C(5)-C(6)-H(5)	118.6
C(53)-H(56B)	0.9800	C(1)-C(6)-H(5)	118.6
C(53)-H(56C)	0.9800	C(2)-C(1)-C(6)	114.9(3)
C(54)-H(57A)	0.9800	C(2)-C(1)-B(1)	124.6(2)
C(54)-H(57B)	0.9800	C(6)-C(1)-B(1)	120.3(2)
C(54)-H(57C)	0.9800	B(1)-C(7)-P(1)	110.97(17)
S-Ni-P(2)	109.79(3)	B(1)-C(7)-H(7A)	109.4
S-Ni-P(1)	151.84(3)	P(1)-C(7)-H(7A)	109.4
P(2)-Ni-P(1)	89.44(3)	B(1)-C(7)-H(7B)	109.4
S-Ni-P(3)	101.54(3)	P(1)-C(7)-H(7B)	109.4
P(2)-Ni-P(3)	107.87(3)	H(7A)-C(7)-H(7B)	108.0
P(1)-Ni-P(3)	91.28(3)	B(1)-C(8)-P(2)	117.87(18)
S-Ni-B(1)	150.82(6)	B(1)-C(8)-H(8A)	107.8
P(2)-Ni-B(1)	61.11(5)	P(2)-C(8)-H(8A)	107.8
P(1)-Ni-B(1)	56.69(5)	B(1)-C(8)-H(8B)	107.8
P(3)-Ni-B(1)	60.42(5)	P(2)-C(8)-H(8B)	107.8
C(7)-P(1)-C(10)	109.03(12)	H(8A)-C(8)-H(8B)	107.2
C(7)-P(1)-C(16)	108.57(12)	B(1)-C(9)-P(3)	117.69(17)
C(10)-P(1)-C(16)	101.79(11)	B(1)-C(9)-H(9A)	107.9
C(7)-P(1)-Ni	113.12(9)	P(3)-C(9)-H(9A)	107.9
C(10)-P(1)-Ni	113.79(8)	B(1)-C(9)-H(9B)	107.9
C(16)-P(1)-Ni	109.85(9)	P(3)-C(9)-H(9B)	107.9
C(22)-P(2)-C(8)	109.72(12)	H(9A)-C(9)-H(9B)	107.2
C(22)-P(2)-C(28)	100.91(12)	C(29)-C(30)-C(31)	120.3(3)
C(8)-P(2)-C(28)	105.11(12)	C(29)-C(30)-H(12)	119.9
C(22)-P(2)-Ni	120.81(9)	C(31)-C(30)-H(12)	119.9
C(8)-P(2)-Ni	102.69(8)	C(32)-C(31)-C(30)	119.6(3)
C(28)-P(2)-Ni	116.73(9)	C(32)-C(31)-H(13)	120.2
C(40)-P(3)-C(9)	108.76(12)	C(30)-C(31)-H(13)	120.2
C(40)-P(3)-C(34)	100.81(11)	C(31)-C(32)-C(33)	120.3(3)
C(9)-P(3)-C(34)	105.73(12)	C(31)-C(32)-H(14)	119.8
C(40)-P(3)-Ni	122.94(9)	C(33)-C(32)-H(14)	119.8
C(9)-P(3)-Ni	107.03(8)	C(28)-C(33)-C(32)	120.4(3)
C(34)-P(3)-Ni	110.35(8)	C(28)-C(33)-H(15)	119.8
C(46)-S-Ni	106.70(9)	C(32)-C(33)-H(15)	119.8
C(1)-B(1)-C(7)	111.0(2)	C(27)-C(22)-C(23)	117.9(3)
C(1)-B(1)-C(8)	110.5(2)	C(27)-C(22)-P(2)	117.7(2)
C(7)-B(1)-C(8)	106.7(2)	C(23)-C(22)-P(2)	124.1(2)
C(1)-B(1)-C(9)	105.5(2)	C(24)-C(23)-C(22)	120.4(3)
C(7)-B(1)-C(9)	110.1(2)	C(24)-C(23)-H(17)	119.8
C(8)-B(1)-C(9)	113.1(2)	C(22)-C(23)-H(17)	119.8
C(1)-B(1)-Ni	175.30(18)	C(25)-C(24)-C(23)	120.6(3)
C(7)-B(1)-Ni	73.72(13)	C(25)-C(24)-H(18)	119.7
C(8)-B(1)-Ni	67.62(13)	C(23)-C(24)-H(18)	119.7
C(9)-B(1)-Ni	72.00(13)	C(26)-C(25)-C(24)	120.1(3)
C(1)-C(2)-C(3)	122.7(3)	C(26)-C(25)-H(19)	120.0
C(1)-C(2)-H(1)	118.6	C(24)-C(25)-H(19)	120.0
C(3)-C(2)-H(1)	118.6	C(25)-C(26)-C(27)	119.6(3)
C(4)-C(3)-C(2)	120.4(3)	C(25)-C(26)-H(20)	120.2
C(4)-C(3)-H(2)	119.8	C(27)-C(26)-H(20)	120.2
C(2)-C(3)-H(2)	119.8	C(26)-C(27)-C(22)	121.5(3)

C(26)-C(27)-H(21)	119.3	C(41)-C(42)-H(40)	120.1
C(22)-C(27)-H(21)	119.3	C(42)-C(41)-C(40)	120.7(3)
C(33)-C(28)-C(29)	118.8(2)	C(42)-C(41)-H(41)	119.7
C(33)-C(28)-P(2)	123.3(2)	C(40)-C(41)-H(41)	119.7
C(29)-C(28)-P(2)	117.9(2)	C(39)-C(34)-C(35)	117.9(2)
C(30)-C(29)-C(28)	120.5(3)	C(39)-C(34)-P(3)	118.9(2)
C(30)-C(29)-H(23)	119.7	C(35)-C(34)-P(3)	123.1(2)
C(28)-C(29)-H(23)	119.7	C(38)-C(39)-C(34)	120.9(3)
C(15)-C(10)-C(11)	118.1(3)	C(38)-C(39)-H(43)	119.5
C(15)-C(10)-P(1)	120.0(2)	C(34)-C(39)-H(43)	119.5
C(11)-C(10)-P(1)	121.9(2)	C(37)-C(38)-C(39)	120.4(3)
C(10)-C(11)-C(12)	121.1(3)	C(37)-C(38)-H(44)	119.8
C(10)-C(11)-H(25)	119.5	C(39)-C(38)-H(44)	119.8
C(12)-C(11)-H(25)	119.5	C(38)-C(37)-C(36)	119.9(3)
C(13)-C(12)-C(11)	119.5(3)	C(38)-C(37)-H(45)	120.1
C(13)-C(12)-H(26)	120.3	C(36)-C(37)-H(45)	120.1
C(11)-C(12)-H(26)	120.3	C(37)-C(36)-C(35)	119.9(3)
C(14)-C(13)-C(12)	120.1(3)	C(37)-C(36)-H(46)	120.1
C(14)-C(13)-H(27)	120.0	C(35)-C(36)-H(46)	120.1
C(12)-C(13)-H(27)	120.0	C(36)-C(35)-C(34)	120.9(3)
C(13)-C(14)-C(15)	120.4(3)	C(36)-C(35)-H(47)	119.5
C(13)-C(14)-H(28)	119.8	C(34)-C(35)-H(47)	119.5
C(15)-C(14)-H(28)	119.8	C(51)-C(46)-C(47)	117.7(3)
C(14)-C(15)-C(10)	120.8(3)	C(51)-C(46)-S	121.7(2)
C(14)-C(15)-H(29)	119.6	C(47)-C(46)-S	120.7(2)
C(10)-C(15)-H(29)	119.6	C(46)-C(51)-C(50)	121.3(3)
C(21)-C(16)-C(17)	118.7(3)	C(46)-C(51)-H(49)	119.3
C(21)-C(16)-P(1)	118.4(2)	C(50)-C(51)-H(49)	119.3
C(17)-C(16)-P(1)	122.8(2)	C(49)-C(50)-C(51)	120.6(3)
C(16)-C(21)-C(20)	121.3(3)	C(49)-C(50)-H(50)	119.7
C(16)-C(21)-H(31)	119.3	C(51)-C(50)-H(50)	119.7
C(20)-C(21)-H(31)	119.3	C(48)-C(49)-C(50)	117.0(3)
C(19)-C(20)-C(21)	119.6(3)	C(48)-C(49)-C(52)	120.4(3)
C(19)-C(20)-H(32)	120.2	C(50)-C(49)-C(52)	122.5(3)
C(21)-C(20)-H(32)	120.2	C(47)-C(48)-C(49)	122.6(3)
C(20)-C(19)-C(18)	119.6(3)	C(47)-C(48)-H(52)	118.7
C(20)-C(19)-H(33)	120.2	C(49)-C(48)-H(52)	118.7
C(18)-C(19)-H(33)	120.2	C(48)-C(47)-C(46)	120.7(3)
C(19)-C(18)-C(17)	121.3(3)	C(48)-C(47)-H(53)	119.6
C(19)-C(18)-H(34)	119.3	C(46)-C(47)-H(53)	119.6
C(17)-C(18)-H(34)	119.3	C(55)-C(52)-C(54)	108.4(3)
C(18)-C(17)-C(16)	119.5(3)	C(55)-C(52)-C(49)	112.8(3)
C(18)-C(17)-H(35)	120.2	C(54)-C(52)-C(49)	110.0(3)
C(16)-C(17)-H(35)	120.2	C(55)-C(52)-C(53)	109.1(3)
C(41)-C(40)-C(45)	118.4(2)	C(54)-C(52)-C(53)	109.4(3)
C(41)-C(40)-P(3)	121.5(2)	C(49)-C(52)-C(53)	107.1(2)
C(45)-C(40)-P(3)	120.1(2)	C(52)-C(55)-H(55A)	109.5
C(44)-C(45)-C(40)	120.3(3)	C(52)-C(55)-H(55B)	109.5
C(44)-C(45)-H(37)	119.8	H(55A)-C(55)-H(55B)	109.5
C(40)-C(45)-H(37)	119.8	C(52)-C(55)-H(55C)	109.5
C(43)-C(44)-C(45)	120.1(3)	H(55A)-C(55)-H(55C)	109.5
C(43)-C(44)-H(38)	119.9	H(55B)-C(55)-H(55C)	109.5
C(45)-C(44)-H(38)	119.9	C(52)-C(53)-H(56A)	109.5
C(42)-C(43)-C(44)	120.6(3)	C(52)-C(53)-H(56B)	109.5
C(42)-C(43)-H(39)	119.7	H(56A)-C(53)-H(56B)	109.5
C(44)-C(43)-H(39)	119.7	C(52)-C(53)-H(56C)	109.5
C(43)-C(42)-C(41)	119.9(3)	H(56A)-C(53)-H(56C)	109.5
C(43)-C(42)-H(40)	120.1	H(56B)-C(53)-H(56C)	109.5

C(52)-C(54)-H(57A)	109.5	C(52)-C(54)-H(57C)	109.5
C(52)-C(54)-H(57B)	109.5	H(57A)-C(54)-H(57C)	109.5
H(57A)-C(54)-H(57B)	109.5	H(57B)-C(54)-H(57C)	109.5

Table 29. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for 7. The anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2 a^{*2} U^{11} + ... + 2\ h\ k\ a^*\ b^*\ U^{12}]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Ni	21(1)	21(1)	20(1)	0(1)	-2(1)	1(1)
P(1)	25(1)	22(1)	21(1)	-1(1)	-3(1)	2(1)
P(2)	22(1)	29(1)	22(1)	4(1)	1(1)	3(1)
P(3)	20(1)	24(1)	20(1)	1(1)	-2(1)	0(1)
S	26(1)	50(1)	31(1)	17(1)	-1(1)	-2(1)
B(1)	22(2)	21(2)	21(2)	1(1)	-3(2)	-2(2)
C(2)	36(2)	25(2)	24(2)	2(1)	4(1)	3(1)
C(3)	43(2)	40(2)	24(2)	9(2)	-1(2)	7(2)
C(4)	33(2)	29(2)	49(2)	16(2)	-6(2)	2(2)
C(5)	53(2)	18(2)	75(3)	0(2)	-32(2)	-3(2)
C(6)	43(2)	27(2)	51(2)	2(2)	-27(2)	5(2)
C(1)	18(2)	23(2)	23(2)	1(1)	2(1)	1(1)
C(7)	25(2)	24(2)	23(2)	4(1)	-2(1)	0(1)
C(8)	16(2)	26(2)	26(2)	1(1)	-3(1)	-4(1)
C(9)	29(2)	21(2)	16(1)	0(1)	-4(1)	-1(1)
C(30)	30(2)	39(2)	29(2)	1(2)	-3(2)	3(2)
C(31)	50(2)	44(2)	18(2)	-1(2)	4(2)	11(2)
C(32)	35(2)	44(2)	31(2)	7(2)	14(2)	8(2)
C(33)	22(2)	37(2)	29(2)	1(1)	1(1)	4(1)
C(22)	22(2)	24(2)	24(2)	2(1)	3(1)	0(1)
C(23)	28(2)	28(2)	60(2)	11(2)	-5(2)	-1(2)
C(24)	24(2)	36(2)	118(3)	15(2)	-13(2)	1(2)
C(25)	24(2)	41(2)	82(3)	5(2)	1(2)	-11(2)
C(26)	38(2)	30(2)	49(2)	8(2)	9(2)	-9(2)
C(27)	29(2)	27(2)	37(2)	5(1)	3(2)	4(1)
C(28)	20(2)	28(2)	24(2)	2(1)	1(1)	6(1)
C(29)	31(2)	36(2)	22(2)	4(1)	6(1)	5(2)
C(10)	32(2)	21(2)	17(2)	1(1)	1(1)	1(1)
C(11)	38(2)	26(2)	29(2)	1(1)	-7(2)	-3(2)
C(12)	37(2)	40(2)	39(2)	4(2)	-9(2)	-8(2)
C(13)	47(2)	26(2)	45(2)	-2(2)	9(2)	-14(2)
C(14)	47(2)	30(2)	48(2)	12(2)	9(2)	2(2)
C(15)	30(2)	27(2)	36(2)	3(2)	1(1)	2(2)
C(16)	24(2)	23(2)	20(2)	-5(1)	-2(1)	-3(1)
C(21)	31(2)	29(2)	26(2)	0(1)	0(1)	0(1)
C(20)	33(2)	37(2)	36(2)	-4(2)	3(2)	6(2)
C(19)	40(2)	41(2)	29(2)	-11(2)	7(2)	-2(2)
C(18)	45(2)	40(2)	27(2)	1(2)	7(2)	-8(2)
C(17)	33(2)	28(2)	26(2)	-2(1)	-1(1)	-1(2)
C(40)	16(2)	31(2)	19(2)	-8(1)	-5(1)	-1(1)
C(45)	27(2)	28(2)	23(2)	-2(1)	-5(1)	0(1)
C(44)	27(2)	34(2)	34(2)	-10(2)	-7(2)	9(2)
C(43)	24(2)	48(2)	34(2)	-16(2)	4(2)	2(2)
C(42)	29(2)	44(2)	29(2)	1(2)	3(1)	-8(2)
C(41)	23(2)	33(2)	29(2)	3(1)	-3(1)	-1(1)
C(34)	18(2)	26(2)	18(2)	1(1)	1(1)	-3(1)
C(39)	31(2)	28(2)	25(2)	3(1)	-2(1)	-2(1)
C(38)	28(2)	34(2)	27(2)	2(2)	-6(1)	-7(2)
C(37)	30(2)	37(2)	25(2)	-9(2)	1(1)	-12(2)
C(36)	32(2)	26(2)	30(2)	-5(1)	4(1)	-3(1)
C(35)	22(2)	29(2)	23(2)	3(1)	-1(1)	-1(1)
C(46)	24(2)	27(2)	36(2)	13(1)	-3(1)	2(1)
C(51)	34(2)	41(2)	25(2)	5(2)	5(2)	6(2)

C(50)	33(2)	33(2)	40(2)	5(2)	4(2)	-2(2)
C(49)	29(2)	28(2)	33(2)	9(2)	7(1)	8(1)
C(48)	45(2)	35(2)	30(2)	1(2)	10(2)	0(2)
C(47)	44(2)	30(2)	36(2)	4(2)	0(2)	3(2)
C(52)	42(2)	38(2)	43(2)	11(2)	16(2)	6(2)
C(55)	65(3)	50(2)	77(3)	3(2)	40(2)	-16(2)
C(53)	53(3)	67(3)	112(3)	28(2)	38(2)	14(2)
C(54)	94(3)	78(3)	49(2)	14(2)	22(2)	-23(3)

Table 30. Hydrogen coordinates (x 10^4) and isotropic displacement parameters (Å^{2}x 10^3) for 7.

	x	y	z	U(eq)
H(1)	4638	53	4651	34
H(2)	4774	-448	5605	42
H(3)	4631	-995	4945	45
H(4)	4338	-1034	3328	59
H(5)	4208	-536	2366	48
H(7A)	4706	538	2950	29
H(7B)	4465	518	3991	29
H(8A)	4219	-28	1100	28
H(8B)	4620	20	1414	28
H(9A)	3795	265	3657	26
H(9B)	3747	-62	2883	26
H(12)	3859	-34	-2313	39
H(13)	4307	75	-3531	45
H(14)	4802	379	-2994	44
H(15)	4854	576	-1244	35
H(17)	5119	291	1181	46
H(18)	5670	542	1020	71
H(19)	5730	1117	473	59
H(20)	5238	1448	81	47
H(21)	4685	1202	247	37
H(23)	3900	176	-581	35
H(25)	4942	1040	3479	38
H(26)	5307	1529	3539	46
H(27)	5102	2067	2920	47
H(28)	4551	2107	2171	50
H(29)	4195	1617	2050	37
H(31)	3697	1418	2949	34
H(32)	3277	1584	4202	42
H(33)	3232	1278	5798	44
H(34)	3616	822	6155	45
H(35)	4050	666	4942	35
H(37)	3130	1053	1917	31
H(38)	2616	1224	2761	38
H(39)	2358	862	4019	42
H(40)	2607	326	4441	41
H(41)	3128	153	3631	34
H(43)	3103	514	288	33
H(44)	2915	164	-1103	36
H(45)	3107	-410	-1243	37
H(46)	3459	-649	88	35
H(47)	3653	-299	1483	30
H(49)	4067	1640	29	40
H(50)	4460	1908	-1139	42
H(52)	4285	1141	-3260	44
H(53)	3895	880	-2124	44
H(55A)	4966	2158	-3314	96
H(55B)	4877	2084	-2090	96
H(55C)	4579	2225	-2873	96
H(56A)	5187	1552	-3548	116
H(56B)	4951	1229	-3166	116
H(56C)	5116	1491	-2307	116
H(57A)	4334	1838	-4264	110
H(57B)	4494	1455	-4428	110
H(57C)	4723	1793	-4709	110

Figure 6. Fully-labeled displacement ellipsoid (50%) representation of $[PhB(CH_2P(O)Ph_2)_2(CH_2PPh_2)]NiCl \cdot C_6H_6$ (**8A · C_6H_6**) (hydrogens omitted for clarity).

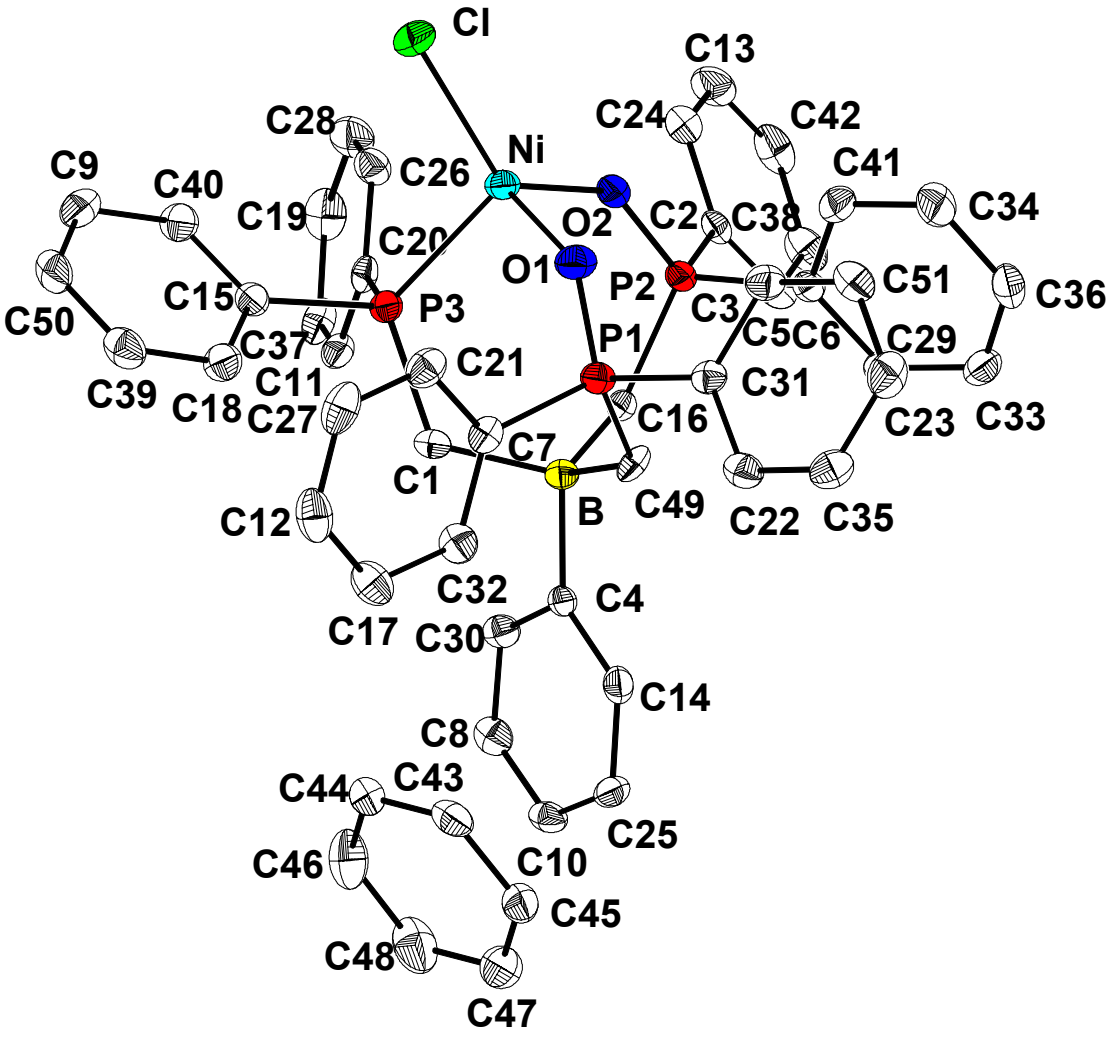


Table 31. Crystal data and structure refinement for 8A · C_6H_6.

Empirical formula	$C_{51}H_{47}BClNiO_2P_3$	
Moiety formula	$C_{45}H_{41}BClNiO_2P_3 \cdot C_6H_6$	
Formula weight	889.77	
Crystal habit	plate	
Crystal color	dichroic	
Crystal size	0.33 x 0.28 x 0.09 mm^3	
Data Collection		
Type of diffractometer	CCD area detector	
Wavelength	0.71073 Å	
Temperature	100(2) K	
Unit cell dimensions	a = 16.2376(12) Å	α = 90°
	b = 16.4690(13) Å	β = 113.3790(10)°
	c = 17.7364(14) Å	γ = 90°
Volume	4353.6(6) $Å^3$	
Z	4	
Crystal system	Monoclinic	
Space group	$P2_1/c$	
Density (calculated)	1.357 g/cm^3	
F(000)	1856	
θ range for data collection	1.76 to 28.44°	
Completeness to θ = 28.44°	93.9%	
Index ranges	$-21 \le h \le 21$, $-21 \le k \le 21$, $-23 \le l \le 23$	
Reflections collected	61180	
Independent reflections	10300 [R(int) = 0.0856]	
Absorption coefficient	0.658 mm^{-1}	
Absorption correction	None	
Structure solution and refinement		
Structure solution program	SHELXS-97 (Sheldrick, 1990)	
Primary solution method	direct methods	
Secondary solution method	difference Fourier map	
Hydrogen placement	calculated positions	
Structure refinement program	SHELXL-97 (Sheldrick, 1997)	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	10300 / 0 / 532	
Goodness-of-fit on F^2	1.601	
Final R indices [$I>2\sigma(I)$]	R1 = 0.0493, wR2 = 0.0732	
R indices (all data)	R1 = 0.0928, wR2 = 0.0784	
Type of weighting scheme used	calculated	
Weighting scheme used	$w=1/[\sigma^2(F_o^2)]$	
Max shift/error	0.008	
Average shift/error	0.001	
Largest diff. peak and hole	1.410 and -0.875 $e \cdot Å^{-3}$	

Table 32. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$ x 10^3) for 8A · C_6H_6. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
Ni	1273(1)	8118(1)	1397(1)	19(1)
P(3)	616(1)	7335(1)	242(1)	17(1)
P(2)	2697(1)	8677(1)	637(1)	17(1)
P(1)	2746(1)	6718(1)	2113(1)	19(1)
Cl	243(1)	8569(1)	1814(1)	28(1)
O(2)	2005(1)	8797(1)	999(1)	21(1)
O(1)	2210(1)	7452(1)	2156(1)	25(1)
B	2445(2)	6846(2)	314(2)	17(1)
C(1)	1376(2)	6609(1)	94(1)	17(1)
C(2)	2658(2)	9554(1)	7(1)	17(1)
C(3)	3918(2)	7359(2)	3585(2)	24(1)
C(4)	2753(2)	6234(1)	-266(2)	17(1)
C(5)	3212(2)	9605(2)	-424(2)	24(1)
C(6)	3807(2)	8723(1)	1454(2)	17(1)
C(7)	2131(2)	5798(2)	2091(1)	19(1)
C(8)	2429(2)	5690(1)	-1644(2)	22(1)
C(9)	-1932(2)	6796(2)	31(2)	31(1)
C(10)	3153(2)	5172(1)	-1341(2)	22(1)
C(11)	76(2)	7733(2)	-1445(2)	22(1)
C(12)	1187(2)	4404(2)	2129(2)	31(1)
C(13)	2061(2)	10873(2)	-511(2)	31(1)
C(14)	3488(2)	5712(2)	8(2)	21(1)
C(15)	-367(2)	6787(1)	230(1)	19(1)
C(16)	2581(2)	7793(1)	25(1)	17(1)
C(17)	1739(2)	4400(2)	1705(2)	29(1)
C(18)	-298(2)	6007(2)	555(2)	24(1)
C(19)	-585(2)	9010(2)	-2020(2)	30(1)
C(20)	170(2)	7986(1)	-665(2)	17(1)
C(21)	1567(2)	5791(2)	2512(2)	25(1)
C(22)	4326(2)	6043(2)	3265(2)	23(1)
C(23)	5279(2)	6722(2)	4487(2)	29(1)
C(24)	2074(2)	10189(2)	-38(2)	27(1)
C(25)	3691(2)	5188(1)	-518(2)	23(1)
C(26)	-113(2)	8770(1)	-577(2)	22(1)
C(27)	1101(2)	5094(2)	2534(2)	30(1)
C(28)	-498(2)	9275(2)	-1253(2)	30(1)
C(29)	4590(2)	8517(1)	1350(2)	22(1)
C(30)	2244(2)	6209(1)	-1118(2)	20(1)
C(31)	3727(2)	6697(1)	3061(2)	18(1)
C(32)	2215(2)	5093(2)	1689(2)	24(1)
C(33)	5419(2)	8612(2)	1984(2)	25(1)
C(34)	4723(2)	9127(2)	2838(2)	33(1)
C(35)	5093(2)	6054(2)	3972(2)	26(1)
C(36)	5485(2)	8915(2)	2728(2)	26(1)
C(37)	-295(2)	8243(2)	-2117(2)	26(1)
C(38)	3191(2)	10291(2)	-880(2)	28(1)
C(39)	-1028(2)	5633(2)	620(2)	28(1)
C(40)	-1194(2)	7174(2)	-30(2)	25(1)
C(41)	3890(2)	9037(2)	2208(2)	27(1)
C(42)	2621(2)	10915(2)	-923(2)	30(1)
C(43)	3500(2)	1906(2)	3696(2)	26(1)
C(44)	2691(2)	2037(2)	3064(2)	28(1)
C(45)	4234(2)	1667(2)	3548(2)	28(1)

C(46)	2606(2)	1935(2)	2266(2)	40(1)
C(47)	4148(2)	1554(2)	2748(2)	37(1)
C(48)	3332(2)	1687(2)	2101(2)	42(1)
C(49)	3121(2)	6696(1)	1303(1)	18(1)
C(50)	-1839(2)	6022(2)	362(2)	30(1)
C(51)	4692(2)	7374(2)	4292(2)	28(1)

Table 33. Selected bond lengths [Å] and angles [°] for 8A · C_6H_6.

Ni-O(1)	1.9255(16)	O(1)-Ni-O(2)	98.80(7)
Ni-O(2)	1.9563(15)	O(1)-Ni-Cl	116.79(5)
Ni-Cl	2.2094(7)	O(2)-Ni-Cl	125.31(5)
Ni-P(3)	2.2944(7)	O(1)-Ni-P(3)	105.21(5)
Ni-B	3.820(3)	O(2)-Ni-P(3)	97.65(5)
		Cl-Ni-P(3)	110.05(3)

Table 34. Bond lengths [Å] and angles [°] for 8A · C_6H_6.

Ni-O(1)	1.9255(16)	C(16)-H(16A)	0.9900
Ni-O(2)	1.9563(15)	C(16)-H(16B)	0.9900
Ni-Cl	2.2094(7)	C(17)-C(32)	1.385(3)
Ni-P(3)	2.2944(7)	C(17)-H(17)	0.9500
Ni-B	3.820(3)	C(18)-C(39)	1.381(3)
P(3)-C(1)	1.811(2)	C(18)-H(18)	0.9500
P(3)-C(15)	1.825(2)	C(19)-C(37)	1.381(3)
P(3)-C(20)	1.826(2)	C(19)-C(28)	1.382(3)
P(2)-O(2)	1.5116(16)	C(19)-H(19)	0.9500
P(2)-C(16)	1.781(2)	C(20)-C(26)	1.399(3)
P(2)-C(6)	1.811(2)	C(21)-C(27)	1.383(3)
P(2)-C(2)	1.812(2)	C(21)-H(21)	0.9500
P(1)-O(1)	1.5085(16)	C(22)-C(35)	1.373(3)
P(1)-C(49)	1.769(2)	C(22)-C(31)	1.399(3)
P(1)-C(31)	1.800(3)	C(22)-H(22)	0.9500
P(1)-C(7)	1.808(2)	C(23)-C(35)	1.384(3)
B-C(4)	1.654(3)	C(23)-C(51)	1.386(3)
B-C(1)	1.667(3)	C(23)-H(23)	0.9500
B-C(49)	1.678(3)	C(24)-H(24)	0.9500
B-C(16)	1.684(3)	C(25)-H(25)	0.9500
C(1)-H(1A)	0.9900	C(26)-C(28)	1.388(3)
C(1)-H(1B)	0.9900	C(26)-H(26)	0.9500
C(2)-C(24)	1.392(3)	C(27)-H(27)	0.9500
C(2)-C(5)	1.395(3)	C(28)-H(28)	0.9500
C(3)-C(51)	1.379(3)	C(29)-C(33)	1.378(3)
C(3)-C(31)	1.386(3)	C(29)-H(29)	0.9500
C(3)-H(3)	0.9500	C(30)-H(30)	0.9500
C(4)-C(14)	1.392(3)	C(32)-H(32)	0.9500
C(4)-C(30)	1.405(3)	C(33)-C(36)	1.374(3)
C(5)-C(38)	1.381(3)	C(33)-H(33)	0.9500
C(5)-H(5)	0.9500	C(34)-C(36)	1.373(3)
C(6)-C(41)	1.389(3)	C(34)-C(41)	1.378(3)
C(6)-C(29)	1.397(3)	C(34)-H(34)	0.9500
C(7)-C(21)	1.393(3)	C(35)-H(35)	0.9500
C(7)-C(32)	1.396(3)	C(36)-H(36)	0.9500
C(8)-C(10)	1.378(3)	C(37)-H(37)	0.9500
C(8)-C(30)	1.383(3)	C(38)-C(42)	1.365(3)
C(8)-H(8)	0.9500	C(38)-H(38)	0.9500
C(9)-C(50)	1.386(3)	C(39)-C(50)	1.370(4)
C(9)-C(40)	1.392(3)	C(39)-H(39)	0.9500
C(9)-H(9)	0.9500	C(40)-H(40)	0.9500
C(10)-C(25)	1.371(3)	C(41)-H(41)	0.9500
C(10)-H(10)	0.9500	C(42)-H(42)	0.9500
C(11)-C(37)	1.386(3)	C(43)-C(44)	1.364(3)
C(11)-C(20)	1.394(3)	C(43)-C(45)	1.376(3)
C(11)-H(11)	0.9500	C(43)-H(43)	0.9500
C(12)-C(27)	1.379(4)	C(44)-C(46)	1.376(4)
C(12)-C(17)	1.381(3)	C(44)-H(44)	0.9500
C(12)-H(12)	0.9500	C(45)-C(47)	1.380(4)
C(13)-C(42)	1.376(3)	C(45)-H(45)	0.9500
C(13)-C(24)	1.399(3)	C(46)-C(48)	1.384(4)
C(13)-H(13)	0.9500	C(46)-H(46)	0.9500
C(14)-C(25)	1.403(3)	C(47)-C(48)	1.384(4)
C(14)-H(14)	0.9500	C(47)-H(47)	0.9500
C(15)-C(40)	1.389(3)	C(48)-H(48)	0.9500
C(15)-C(18)	1.395(3)	C(49)-H(49A)	0.9900

C(49)-H(49B)	0.9900
C(50)-H(50)	0.9500
C(51)-H(51)	0.9500
O(1)-Ni-O(2)	98.80(7)
O(1)-Ni-Cl	116.79(5)
O(2)-Ni-Cl	125.31(5)
O(1)-Ni-P(3)	105.21(5)
O(2)-Ni-P(3)	97.65(5)
Cl-Ni-P(3)	110.05(3)
O(1)-Ni-B	68.03(6)
O(2)-Ni-B	68.71(6)
Cl-Ni-B	161.29(5)
P(3)-Ni-B	52.47(5)
C(1)-P(3)-C(15)	108.33(11)
C(1)-P(3)-C(20)	108.40(11)
C(15)-P(3)-C(20)	103.94(11)
C(1)-P(3)-Ni	113.49(8)
C(15)-P(3)-Ni	112.48(8)
C(20)-P(3)-Ni	109.71(8)
O(2)-P(2)-C(16)	116.75(10)
O(2)-P(2)-C(6)	109.02(10)
C(16)-P(2)-C(6)	110.63(11)
O(2)-P(2)-C(2)	107.91(10)
C(16)-P(2)-C(2)	107.82(11)
C(6)-P(2)-C(2)	103.88(11)
O(1)-P(1)-C(49)	116.72(10)
O(1)-P(1)-C(31)	106.45(10)
C(49)-P(1)-C(31)	107.27(11)
O(1)-P(1)-C(7)	110.33(11)
C(49)-P(1)-C(7)	109.24(11)
C(31)-P(1)-C(7)	106.25(11)
P(2)-O(2)-Ni	137.62(10)
P(1)-O(1)-Ni	137.14(10)
C(4)-B-C(1)	104.80(19)
C(4)-B-C(49)	109.04(19)
C(1)-B-C(49)	113.52(19)
C(4)-B-C(16)	105.37(18)
C(1)-B-C(16)	113.40(19)
C(49)-B-C(16)	110.17(19)
C(4)-B-Ni	168.87(16)
C(1)-B-Ni	64.32(11)
C(49)-B-Ni	78.80(12)
C(16)-B-Ni	78.33(12)
B-C(1)-P(3)	121.11(16)
B-C(1)-H(1A)	107.0
P(3)-C(1)-H(1A)	107.0
B-C(1)-H(1B)	107.0
P(3)-C(1)-H(1B)	107.0
H(1A)-C(1)-H(1B)	106.8
C(24)-C(2)-C(5)	119.7(2)
C(24)-C(2)-P(2)	119.40(19)
C(5)-C(2)-P(2)	120.93(19)
C(51)-C(3)-C(31)	120.3(2)
C(51)-C(3)-H(3)	119.9
C(31)-C(3)-H(3)	119.9
C(14)-C(4)-C(30)	114.5(2)
C(14)-C(4)-B	126.0(2)
C(30)-C(4)-B	119.5(2)
C(38)-C(5)-C(2)	120.0(2)
C(38)-C(5)-H(5)	120.0
C(2)-C(5)-H(5)	120.0
C(41)-C(6)-C(29)	118.0(2)
C(41)-C(6)-P(2)	118.14(19)
C(29)-C(6)-P(2)	123.64(19)
C(21)-C(7)-C(32)	119.0(2)
C(21)-C(7)-P(1)	118.06(19)
C(32)-C(7)-P(1)	122.89(19)
C(10)-C(8)-C(30)	120.0(2)
C(10)-C(8)-H(8)	120.0
C(30)-C(8)-H(8)	120.0
C(50)-C(9)-C(40)	119.5(2)
C(50)-C(9)-H(9)	120.3
C(40)-C(9)-H(9)	120.3
C(25)-C(10)-C(8)	119.1(2)
C(25)-C(10)-H(10)	120.4
C(8)-C(10)-H(10)	120.4
C(37)-C(11)-C(20)	120.8(2)
C(37)-C(11)-H(11)	119.6
C(20)-C(11)-H(11)	119.6
C(27)-C(12)-C(17)	120.6(3)
C(27)-C(12)-H(12)	119.7
C(17)-C(12)-H(12)	119.7
C(42)-C(13)-C(24)	120.2(3)
C(42)-C(13)-H(13)	119.9
C(24)-C(13)-H(13)	119.9
C(4)-C(14)-C(25)	122.8(2)
C(4)-C(14)-H(14)	118.6
C(25)-C(14)-H(14)	118.6
C(40)-C(15)-C(18)	117.9(2)
C(40)-C(15)-P(3)	120.20(19)
C(18)-C(15)-P(3)	121.61(19)
B-C(16)-P(2)	124.45(16)
B-C(16)-H(16A)	106.2
P(2)-C(16)-H(16A)	106.2
B-C(16)-H(16B)	106.2
P(2)-C(16)-H(16B)	106.2
H(16A)-C(16)-H(16B)	106.4
C(12)-C(17)-C(32)	119.7(3)
C(12)-C(17)-H(17)	120.2
C(32)-C(17)-H(17)	120.2
C(39)-C(18)-C(15)	121.0(2)
C(39)-C(18)-H(18)	119.5
C(15)-C(18)-H(18)	119.5
C(37)-C(19)-C(28)	120.3(2)
C(37)-C(19)-H(19)	119.9
C(28)-C(19)-H(19)	119.9
C(11)-C(20)-C(26)	118.3(2)
C(11)-C(20)-P(3)	123.16(19)
C(26)-C(20)-P(3)	118.51(18)
C(27)-C(21)-C(7)	120.3(2)
C(27)-C(21)-H(21)	119.8
C(7)-C(21)-H(21)	119.8
C(35)-C(22)-C(31)	120.7(2)
C(35)-C(22)-H(22)	119.6
C(31)-C(22)-H(22)	119.6

C(35)-C(23)-C(51)	120.2(3)	C(42)-C(38)-C(5)	120.4(3)
C(35)-C(23)-H(23)	119.9	C(42)-C(38)-H(38)	119.8
C(51)-C(23)-H(23)	119.9	C(5)-C(38)-H(38)	119.8
C(2)-C(24)-C(13)	119.2(2)	C(50)-C(39)-C(18)	120.5(2)
C(2)-C(24)-H(24)	120.4	C(50)-C(39)-H(39)	119.7
C(13)-C(24)-H(24)	120.4	C(18)-C(39)-H(39)	119.7
C(10)-C(25)-C(14)	120.1(2)	C(15)-C(40)-C(9)	121.2(2)
C(10)-C(25)-H(25)	120.0	C(15)-C(40)-H(40)	119.4
C(14)-C(25)-H(25)	120.0	C(9)-C(40)-H(40)	119.4
C(28)-C(26)-C(20)	120.8(2)	C(34)-C(41)-C(6)	120.7(2)
C(28)-C(26)-H(26)	119.6	C(34)-C(41)-H(41)	119.7
C(20)-C(26)-H(26)	119.6	C(6)-C(41)-H(41)	119.7
C(12)-C(27)-C(21)	120.0(3)	C(38)-C(42)-C(13)	120.6(3)
C(12)-C(27)-H(27)	120.0	C(38)-C(42)-H(42)	119.7
C(21)-C(27)-H(27)	120.0	C(13)-C(42)-H(42)	119.7
C(19)-C(28)-C(26)	119.7(2)	C(44)-C(43)-C(45)	120.9(2)
C(19)-C(28)-H(28)	120.1	C(44)-C(43)-H(43)	119.6
C(26)-C(28)-H(28)	120.1	C(45)-C(43)-H(43)	119.6
C(33)-C(29)-C(6)	120.7(2)	C(43)-C(44)-C(46)	119.8(3)
C(33)-C(29)-H(29)	119.6	C(43)-C(44)-H(44)	120.1
C(6)-C(29)-H(29)	119.6	C(46)-C(44)-H(44)	120.1
C(8)-C(30)-C(4)	123.4(2)	C(43)-C(45)-C(47)	119.5(3)
C(8)-C(30)-H(30)	118.3	C(43)-C(45)-H(45)	120.3
C(4)-C(30)-H(30)	118.3	C(47)-C(45)-H(45)	120.3
C(3)-C(31)-C(22)	119.0(2)	C(44)-C(46)-C(48)	120.4(3)
C(3)-C(31)-P(1)	119.36(19)	C(44)-C(46)-H(46)	119.8
C(22)-C(31)-P(1)	121.54(19)	C(48)-C(46)-H(46)	119.8
C(17)-C(32)-C(7)	120.4(2)	C(45)-C(47)-C(48)	120.3(3)
C(17)-C(32)-H(32)	119.8	C(45)-C(47)-H(47)	119.9
C(7)-C(32)-H(32)	119.8	C(48)-C(47)-H(47)	119.9
C(36)-C(33)-C(29)	120.3(2)	C(47)-C(48)-C(46)	119.1(3)
C(36)-C(33)-H(33)	119.9	C(47)-C(48)-H(48)	120.4
C(29)-C(33)-H(33)	119.9	C(46)-C(48)-H(48)	120.4
C(36)-C(34)-C(41)	120.5(2)	B-C(49)-P(1)	123.52(16)
C(36)-C(34)-H(34)	119.8	B-C(49)-H(49A)	106.4
C(41)-C(34)-H(34)	119.8	P(1)-C(49)-H(49A)	106.4
C(22)-C(35)-C(23)	119.7(2)	B-C(49)-H(49B)	106.4
C(22)-C(35)-H(35)	120.2	P(1)-C(49)-H(49B)	106.4
C(23)-C(35)-H(35)	120.2	H(49A)-C(49)-H(49B)	106.5
C(34)-C(36)-C(33)	119.8(3)	C(39)-C(50)-C(9)	119.9(2)
C(34)-C(36)-H(36)	120.1	C(39)-C(50)-H(50)	120.0
C(33)-C(36)-H(36)	120.1	C(9)-C(50)-H(50)	120.0
C(19)-C(37)-C(11)	120.1(2)	C(3)-C(51)-C(23)	120.1(2)
C(19)-C(37)-H(37)	120.0	C(3)-C(51)-H(51)	119.9
C(11)-C(37)-H(37)	120.0	C(23)-C(51)-H(51)	119.9

Table 35. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for 8A · C_6H_6. The anisotropic displacement factor exponent takes the form: $-2\pi^2[\ h^2 a^{*2} U^{11} + ... + 2\ h\ k\ a^*\ b^*\ U^{12}]$

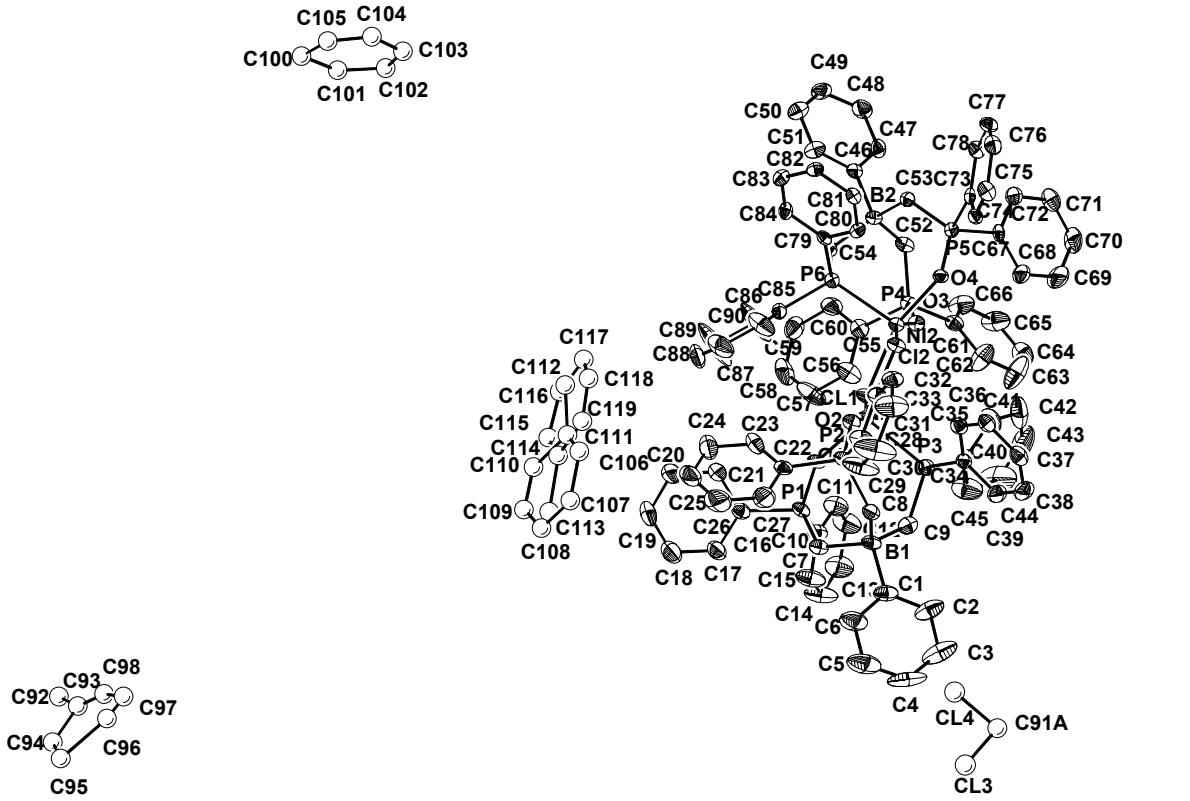
	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Ni	21(1)	16(1)	23(1)	-1(1)	12(1)	0(1)
P(3)	18(1)	15(1)	22(1)	1(1)	11(1)	-1(1)
P(2)	18(1)	14(1)	21(1)	-2(1)	10(1)	-2(1)
P(1)	20(1)	18(1)	20(1)	-2(1)	9(1)	0(1)
Cl	25(1)	32(1)	32(1)	-4(1)	16(1)	4(1)
O(2)	21(1)	17(1)	27(1)	-4(1)	12(1)	-4(1)
O(1)	25(1)	25(1)	21(1)	-2(1)	7(1)	5(1)
B	18(2)	14(2)	18(2)	0(1)	8(1)	1(1)
C(1)	23(1)	13(1)	17(1)	1(1)	12(1)	1(1)
C(2)	18(1)	14(1)	16(1)	-2(1)	2(1)	-3(1)
C(3)	24(2)	20(2)	28(2)	1(1)	10(1)	3(1)
C(4)	17(1)	11(1)	26(2)	-1(1)	13(1)	-4(1)
C(5)	28(2)	20(2)	22(2)	-1(1)	9(1)	-1(1)
C(6)	19(1)	11(1)	21(2)	1(1)	9(1)	-1(1)
C(7)	18(1)	23(2)	17(2)	3(1)	7(1)	2(1)
C(8)	28(2)	19(1)	22(2)	1(1)	14(1)	-5(1)
C(9)	24(2)	30(2)	43(2)	-3(1)	18(1)	2(1)
C(10)	31(2)	16(1)	29(2)	-4(1)	21(1)	-4(1)
C(11)	17(1)	21(2)	30(2)	0(1)	12(1)	0(1)
C(12)	27(2)	31(2)	30(2)	9(1)	6(1)	-9(1)
C(13)	32(2)	17(2)	35(2)	0(1)	3(2)	5(1)
C(14)	17(1)	24(2)	23(2)	-4(1)	8(1)	-6(1)
C(15)	21(1)	19(1)	21(2)	-2(1)	12(1)	-3(1)
C(16)	15(1)	18(1)	19(1)	-3(1)	9(1)	-2(1)
C(17)	36(2)	24(2)	26(2)	0(1)	11(1)	-6(1)
C(18)	24(2)	22(2)	29(2)	2(1)	13(1)	0(1)
C(19)	30(2)	30(2)	29(2)	12(1)	10(1)	-2(1)
C(20)	12(1)	20(1)	20(2)	2(1)	7(1)	-2(1)
C(21)	21(2)	31(2)	21(2)	3(1)	8(1)	4(1)
C(22)	28(2)	21(2)	22(2)	-3(1)	12(1)	-2(1)
C(23)	22(2)	39(2)	20(2)	3(1)	2(1)	2(1)
C(24)	25(2)	23(2)	33(2)	-7(1)	10(1)	-4(1)
C(25)	20(2)	17(1)	37(2)	-2(1)	16(1)	2(1)
C(26)	25(2)	17(1)	23(2)	0(1)	8(1)	-2(1)
C(27)	22(2)	44(2)	28(2)	11(1)	13(1)	0(1)
C(28)	34(2)	17(2)	36(2)	3(1)	12(2)	1(1)
C(29)	25(2)	22(2)	21(2)	-1(1)	11(1)	2(1)
C(30)	24(2)	15(1)	25(2)	2(1)	14(1)	0(1)
C(31)	21(1)	18(1)	18(1)	1(1)	11(1)	0(1)
C(32)	25(2)	25(2)	22(2)	1(1)	12(1)	-2(1)
C(33)	21(2)	21(2)	36(2)	3(1)	15(1)	4(1)
C(34)	28(2)	47(2)	21(2)	-15(1)	7(1)	-5(2)
C(35)	27(2)	27(2)	25(2)	6(1)	10(1)	9(1)
C(36)	20(2)	26(2)	27(2)	0(1)	4(1)	-6(1)
C(37)	17(1)	38(2)	22(2)	3(1)	8(1)	-2(1)
C(38)	37(2)	25(2)	22(2)	0(1)	12(1)	-7(1)
C(39)	36(2)	21(2)	32(2)	-1(1)	19(2)	-8(1)
C(40)	27(2)	22(2)	31(2)	0(1)	18(1)	-3(1)
C(41)	20(2)	34(2)	29(2)	-8(1)	13(1)	-1(1)
C(42)	34(2)	21(2)	23(2)	4(1)	0(1)	-6(1)
C(43)	34(2)	20(2)	28(2)	-6(1)	15(1)	-5(1)
C(44)	24(2)	24(2)	35(2)	-7(1)	10(1)	-4(1)
C(45)	22(2)	23(2)	36(2)	-2(1)	8(1)	-2(1)

C(46)	27(2)	50(2)	33(2)	2(2)	1(2)	-8(2)
C(47)	35(2)	36(2)	51(2)	-12(2)	29(2)	-10(1)
C(48)	45(2)	55(2)	31(2)	-13(2)	21(2)	-20(2)
C(49)	20(1)	13(1)	25(2)	2(1)	12(1)	0(1)
C(50)	32(2)	32(2)	39(2)	-10(1)	26(2)	-16(1)
C(51)	31(2)	25(2)	25(2)	-4(1)	9(1)	-4(1)

Table 36. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for 8A · C_6H_6.

	x	y	z	U(eq)
H(1A)	1377	6121	422	20
H(1B)	1108	6442	-490	20
H(3)	3513	7805	3457	29
H(5)	3603	9169	-404	28
H(8)	2056	5690	-2214	26
H(9)	-2494	7067	-153	37
H(10)	3278	4807	-1697	27
H(11)	268	7205	-1516	27
H(12)	863	3928	2143	37
H(13)	1665	11309	-547	37
H(14)	3868	5710	576	26
H(16A)	2064	7895	-500	20
H(16B)	3120	7775	-106	20
H(17)	1793	3924	1425	35
H(18)	260	5729	736	29
H(19)	-844	9356	-2483	36
H(21)	1501	6267	2785	30
H(22)	4202	5587	2909	28
H(23)	5811	6734	4975	35
H(24)	1689	10158	248	33
H(25)	4202	4845	-304	28
H(26)	-41	8958	-49	27
H(27)	722	5091	2827	36
H(28)	-701	9801	-1189	36
H(29)	4551	8310	837	27
H(30)	1748	6567	-1344	24
H(32)	2601	5089	1403	28
H(33)	5946	8467	1907	29
H(34)	4769	9338	3352	39
H(35)	5494	5606	4108	31
H(36)	6057	8977	3165	32
H(37)	-351	8065	-2644	31
H(38)	3576	10328	-1166	34
H(39)	-968	5102	844	34
H(40)	-1257	7705	-253	30
H(41)	3368	9192	2290	32
H(42)	2611	11383	-1239	35
H(43)	3557	1980	4245	32
H(44)	2188	2198	3174	34
H(45)	4796	1580	3992	33
H(46)	2045	2035	1825	48
H(47)	4651	1385	2642	44
H(48)	3271	1610	1550	50
H(49A)	3606	7104	1440	22
H(49B)	3406	6159	1331	22
H(50)	-2338	5762	411	37
H(51)	4822	7832	4646	33

Figure 7. Fully-labeled displacement ellipsoid (50%) representation of $\{[PhB(CH_2P(O)Ph_2)_2(CH_2PPh_2)]NiCl\}_2 \cdot C_6H_6 \cdot 2\ C_7H_8 \cdot CH_2Cl_{1.5}$ (**8B · C_6H_6· 2 C_7H_8 · $CH_2Cl_{1.5}$**) (hydrogens omitted for clarity).



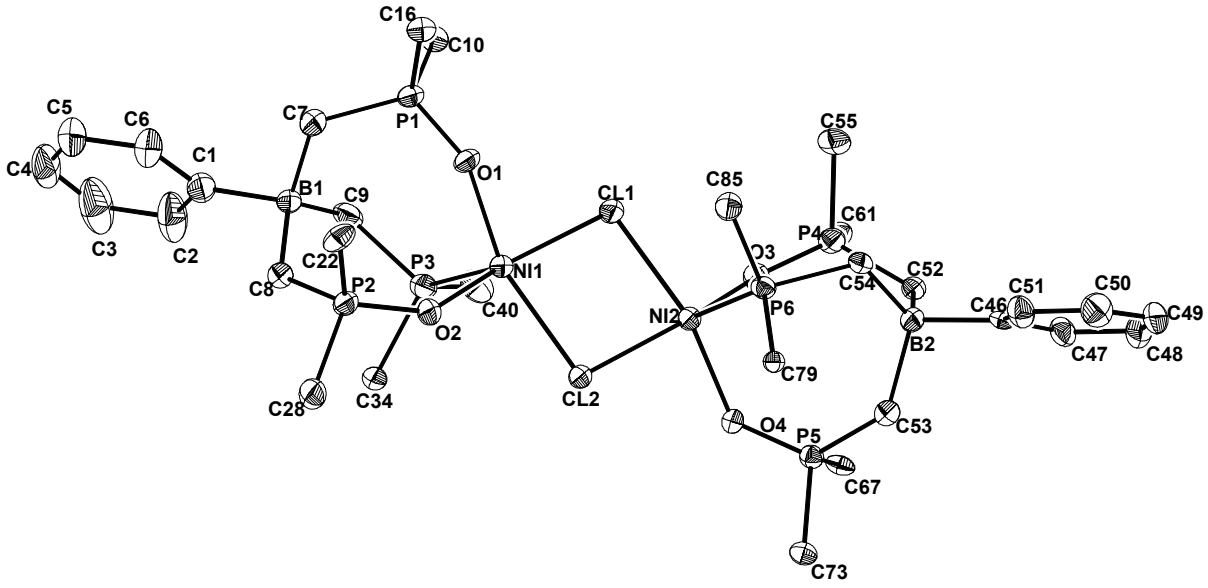


Table 37. Crystal data and structure refinement for 8B · C_6H_6· 2 C_7H_8 · $CH_2Cl_{1.5}$.

Empirical formula	$C_{111}H_{106}B_2Cl_{3.50}Ni_2O_4P_6$	
Moiety formula	$C_{90}H_{82}B_2Cl_2Ni_2O_4P_6$, C_7H_8, C_7H_8, C_6H_6, $CH_2Cl_{1.5}$	
Formula weight	1952.89	
Crystal habit	square plate	
Crystal color	yellow	
Crystal size	0.31 x 0.11 x 0.07 mm^3	
Data Collection		
Type of diffractometer	CCD area detector	
Wavelength	0.71073 Å	
Temperature	98(2) K	
Unit cell dimensions	a = 24.8113(15) Å	α = 90°
	b = 13.9514(8) Å	β = 112.5030(10)°
	c = 30.9581(19) Å	γ = 90°
Volume	9900.3(10) $Å^3$	
Z	4	
Crystal system	Monoclinic	
Space group	$P2_1/n$	
Density (calculated)	1.310 g/cm^3	
F(000)	4078	
θ range for data collection	1.42 to 28.77°	
Completeness to θ = 28.77°	91.4%	
Index ranges	$-31 \le h \le 33$, $-18 \le k \le 18$, $-41 \le l \le 41$	
Reflections collected	108035	
Independent reflections	23533 [R(int) = 0.1185]	
Absorption coefficient	0.625 mm^{-1}	
Absorption correction	None	
Structure solution and refinement		
Structure solution program	SHELXS-97 (Sheldrick, 1990)	
Primary solution method	direct methods	
Secondary solution method	difference Fourier map	
Hydrogen placement	calculated positions	
Structure refinement program	SHELXL-97 (Sheldrick, 1997)	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	23533 / 0 / 1230	
Goodness-of-fit on F^2	1.629	
Final R indices [$I>2\sigma(I)$]	R1 = 0.0697, wR2 = 0.1129	
R indices (all data)	R1 = 0.1489, wR2 = 0.1227	
Type of weighting scheme used	calculated	
Weighting scheme used	$w=1/[\sigma^2(F_o^2)]$	
Max shift/error	8.613	
Average shift/error	0.289	
Largest diff. peak and hole	2.350 and -1.155 $e \cdot Å^{-3}$	

Additional refinement details: The structure contained several disorder solvent molecules: two toluenes, one benzene, and one dichloromethane molecule. One toluene molecule and the dichloromethane molecule were disordered over two positions. In addition, a chlorine atom of the dichloromethane molecule is on a special position of symmetry in the lattice. Overall, the core dinickel molecule refined well. The solvent molecules refined somewhat poorly: attempts to apply constraints resulted in unstable refinements. Although the disorder of the solvent molecules results in a decrease in structural quality, the more significant dinickel molecule is well-defined.

Table 38. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$ x 10^3) for 8B · C_6H_6· 2 C_7H_8 · $CH_2Cl_{1.5}$. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
Ni(1)	3109(1)	6627(1)	518(1)	19(1)
P(1)	2077(1)	6280(1)	967(1)	23(1)
P(2)	2147(1)	5206(1)	-217(1)	24(1)
P(3)	2509(1)	7821(1)	67(1)	23(1)
O(1)	2640(1)	6229(2)	890(1)	22(1)
O(2)	2754(1)	5585(2)	58(1)	23(1)
Cl(1)	3731(1)	7480(1)	1176(1)	24(1)
B(1)	1398(2)	6793(4)	-26(2)	24(1)
Ni(2)	4552(1)	7476(1)	983(1)	18(1)
P(4)	5315(1)	8980(1)	1852(1)	21(1)
P(5)	5730(1)	7956(1)	802(1)	18(1)
P(6)	5098(1)	6264(1)	1470(1)	19(1)
O(3)	4869(1)	8613(2)	1400(1)	23(1)
O(4)	5084(1)	7786(2)	662(1)	19(1)
Cl(2)	3942(1)	6589(1)	314(1)	22(1)
B(2)	6181(2)	7499(4)	1859(2)	20(1)
C(1)	707(2)	7060(4)	-321(2)	35(1)
C(2)	513(2)	7863(4)	-604(2)	53(2)
C(3)	-80(3)	8025(5)	-859(2)	69(2)
C(4)	-497(2)	7392(6)	-847(2)	68(2)
C(5)	-322(2)	6595(6)	-577(2)	69(2)
C(6)	271(2)	6427(5)	-320(2)	55(2)
C(7)	1429(2)	6218(3)	459(1)	26(1)
C(8)	1552(2)	6036(3)	-376(1)	26(1)
C(9)	1796(2)	7801(3)	100(2)	28(1)
C(10)	2050(2)	7355(4)	1286(1)	28(1)
C(11)	2528(2)	7929(4)	1477(2)	40(1)
C(12)	2519(2)	8722(4)	1734(2)	50(2)
C(13)	2033(2)	8954(4)	1817(2)	51(2)
C(14)	1546(2)	8392(5)	1629(2)	54(2)
C(15)	1549(2)	7609(4)	1366(2)	45(2)
C(16)	2064(2)	5336(4)	1359(2)	27(1)
C(17)	1546(2)	5049(4)	1397(2)	39(1)
C(18)	1537(2)	4373(4)	1708(2)	51(2)
C(19)	2049(2)	3940(5)	1984(2)	60(2)
C(20)	2572(2)	4208(5)	1951(2)	56(2)
C(21)	2581(2)	4898(4)	1642(2)	41(1)
C(22)	2012(2)	4214(3)	104(2)	27(1)
C(23)	2426(2)	3969(4)	533(2)	34(1)
C(24)	2356(3)	3188(4)	783(2)	48(2)
C(25)	1860(3)	2641(4)	598(2)	62(2)
C(26)	1442(3)	2880(5)	185(3)	73(2)
C(27)	1505(2)	3656(4)	-69(2)	55(2)
C(28)	2146(2)	4706(4)	-751(2)	31(1)
C(29)	1633(2)	4356(5)	-1100(2)	61(2)
C(30)	1643(2)	3982(6)	-1511(2)	78(2)
C(31)	2157(2)	3978(5)	-1594(2)	58(2)
C(32)	2658(2)	4332(4)	-1255(2)	33(1)
C(33)	2655(2)	4678(3)	-838(2)	26(1)
C(34)	2366(2)	7792(3)	-557(1)	22(1)
C(35)	2652(2)	7162(3)	-733(2)	26(1)
C(36)	2517(2)	7114(3)	-1215(2)	27(1)
C(37)	2087(2)	7691(4)	-1519(2)	31(1)

C(38)	1807(2)	8339(4)	-1340(2)	38(1)
C(39)	1939(2)	8392(4)	-868(2)	34(1)
C(40)	2824(2)	9007(4)	232(2)	31(1)
C(41)	3305(2)	9245(4)	131(2)	45(2)
C(42)	3579(3)	10130(5)	265(2)	59(2)
C(43)	3371(3)	10780(5)	494(2)	74(2)
C(44)	2914(3)	10540(5)	606(3)	102(3)
C(45)	2636(2)	9646(4)	474(2)	64(2)
C(46)	6849(2)	7236(3)	2219(1)	20(1)
C(47)	7280(2)	7937(4)	2381(1)	27(1)
C(48)	7847(2)	7729(4)	2695(2)	35(1)
C(49)	7998(2)	6808(4)	2858(2)	32(1)
C(50)	7596(2)	6092(4)	2690(2)	35(1)
C(51)	7033(2)	6306(3)	2374(2)	28(1)
C(52)	6045(2)	8644(3)	1967(1)	22(1)
C(53)	6216(2)	7422(3)	1327(1)	19(1)
C(54)	5720(2)	6735(3)	1952(1)	19(1)
C(55)	5129(2)	8628(3)	2339(2)	26(1)
C(56)	4536(2)	8531(4)	2254(2)	39(1)
C(57)	4360(3)	8260(5)	2611(2)	54(2)
C(58)	4759(3)	8088(4)	3050(2)	51(2)
C(59)	5348(3)	8179(4)	3141(2)	46(2)
C(60)	5534(2)	8450(4)	2789(2)	36(1)
C(61)	5260(2)	10272(3)	1849(2)	25(1)
C(62)	4780(2)	10717(4)	1519(2)	48(2)
C(63)	4730(3)	11699(4)	1521(2)	66(2)
C(64)	5146(2)	12246(4)	1853(2)	45(2)
C(65)	5610(2)	11820(4)	2176(2)	51(2)
C(66)	5674(2)	10837(4)	2178(2)	44(2)
C(67)	5877(2)	9228(3)	826(1)	19(1)
C(68)	5402(2)	9852(4)	670(2)	36(1)
C(69)	5504(2)	10830(4)	681(2)	54(2)
C(70)	6063(2)	11187(4)	828(2)	44(1)
C(71)	6532(2)	10581(4)	983(2)	36(1)
C(72)	6443(2)	9603(3)	982(2)	30(1)
C(73)	5923(2)	7486(3)	336(1)	18(1)
C(74)	5483(2)	7142(3)	-71(1)	20(1)
C(75)	5620(2)	6727(3)	-419(2)	27(1)
C(76)	6197(2)	6644(3)	-370(2)	29(1)
C(77)	6634(2)	7001(3)	25(2)	26(1)
C(78)	6502(2)	7404(3)	377(1)	23(1)
C(79)	5403(2)	5358(3)	1200(1)	17(1)
C(80)	5353(2)	5459(3)	740(1)	19(1)
C(81)	5622(2)	4814(3)	542(1)	20(1)
C(82)	5931(2)	4046(3)	802(1)	21(1)
C(83)	5969(2)	3925(3)	1256(2)	25(1)
C(84)	5718(2)	4576(3)	1457(1)	22(1)
C(85)	4704(2)	5533(3)	1742(2)	23(1)
C(86)	4355(2)	4792(4)	1497(2)	48(2)
C(87)	4071(3)	4208(4)	1699(3)	63(2)
C(88)	4115(2)	4343(5)	2136(2)	66(2)
C(89)	4447(3)	5076(7)	2377(2)	122(4)
C(90)	4735(3)	5664(6)	2173(2)	86(3)
C(91A)	534(11)	9409(18)	490(6)	350(20)
C(91B)	630(11)	10450(40)	-240(30)	1140(110)
Cl(3)	1086(5)	10025(11)	521(5)	636(10)
Cl(4)	0	10000	0	518(11)
C(92)	1938(5)	1329(9)	9331(4)	252(9)

C(100)	10015(3)	2781(12)	9103(6)	187(7)
C(101)	9999(3)	3856(10)	9137(3)	105(3)
C(102)	9990(2)	4506(7)	8762(3)	82(3)
C(103)	9995(3)	4142(8)	8318(4)	123(4)
C(104)	10017(4)	3152(12)	8255(6)	204(9)
C(105)	10021(4)	2636(10)	8635(7)	154(7)
C(106)	2368(12)	1349(17)	1725(9)	74(7)
C(107)	1701(10)	1266(18)	1601(8)	106(9)
C(108)	1485(14)	1260(30)	1956(16)	98(12)
C(109)	1867(10)	1315(18)	2368(7)	76(7)
C(110)	2420(9)	1369(12)	2438(9)	46(5)
C(111)	2699(10)	1430(20)	2056(12)	55(8)
C(112)	3374(14)	1330(20)	2251(9)	80(9)
C(113)	1751(9)	1501(17)	2056(11)	85(8)
C(114)	2467(13)	1434(14)	2119(8)	69(6)
C(115)	2835(9)	1609(12)	2478(6)	105(6)
C(116)	3418(8)	1610(16)	2495(8)	104(7)
C(117)	3662(11)	1430(20)	2122(13)	150(11)
C(118)	3280(20)	1190(30)	1797(18)	340(30)
C(119)	2705(6)	1162(8)	1690(4)	370(50)
C(93)	1638(6)	1166(8)	8869(4)	190(7)
C(94)	1081(6)	624(8)	8773(4)	280(16)
C(95)	687(9)	289(12)	8347(8)	490(20)
C(96)	1116(8)	673(10)	8000(4)	524(11)
C(97)	1404(6)	881(8)	7957(4)	253(8)
C(98)	1675(6)	1209(10)	8511(4)	177(6)

Table 39. Selected bond lengths [Å] and angles [°] for 8B · C_6H_6· 2 C_7H_8 · $CH_2Cl_{1.5}$.

Ni(1)-O(2)	1.989(3)	O(2)-Ni(1)-O(1)	90.82(12)
Ni(1)-O(1)	2.005(3)	O(2)-Ni(1)-P(3)	95.05(9)
Ni(1)-P(3)	2.3125(13)	O(1)-Ni(1)-P(3)	99.50(9)
Ni(1)-Cl(1)	2.3543(11)	O(2)-Ni(1)-Cl(1)	162.37(9)
Ni(1)-Cl(2)	2.3814(12)	O(1)-Ni(1)-Cl(1)	88.57(8)
Ni(1)-B(1)	3.929(5)	P(3)-Ni(1)-Cl(1)	102.43(5)
Cl(1)-Ni(2)	2.3311(12)	O(2)-Ni(1)-Cl(2)	89.14(9)
Ni(2)-O(4)	1.980(3)	O(1)-Ni(1)-Cl(2)	154.17(9)
Ni(2)-O(3)	2.006(3)	P(3)-Ni(1)-Cl(2)	106.23(5)
Ni(2)-P(6)	2.3236(13)	Cl(1)-Ni(1)-Cl(2)	83.84(4)
Ni(2)-Cl(2)	2.3916(11)	Ni(2)-Cl(1)-Ni(1)	97.20(4)
Ni(2)-B(2)	3.912(4)	O(4)-Ni(2)-O(3)	88.71(11)
		O(4)-Ni(2)-P(6)	98.62(8)
		O(3)-Ni(2)-P(6)	99.80(8)
		O(4)-Ni(2)-Cl(1)	160.59(8)
		O(3)-Ni(2)-Cl(1)	89.98(9)
		P(6)-Ni(2)-Cl(1)	100.69(5)
		O(4)-Ni(2)-Cl(2)	90.03(8)
		O(3)-Ni(2)-Cl(2)	158.33(9)
		P(6)-Ni(2)-Cl(2)	101.78(4)
		Cl(1)-Ni(2)-Cl(2)	84.11(4)
		Ni(1)-Cl(2)-Ni(2)	94.84(4)

Table 40. Bond lengths [Å] and angles [°] for 8B · C_6H_6· 2 C_7H_8 · $CH_2Cl_{1.5}$.

Ni(1)-O(2)	1.989(3)	C(8)-H(8B)	0.9900
Ni(1)-O(1)	2.005(3)	C(9)-H(9A)	0.9900
Ni(1)-P(3)	2.3125(13)	C(9)-H(9B)	0.9900
Ni(1)-Cl(1)	2.3543(11)	C(10)-C(11)	1.365(6)
Ni(1)-Cl(2)	2.3814(12)	C(10)-C(15)	1.404(6)
Ni(1)-B(1)	3.929(5)	C(11)-C(12)	1.368(7)
P(1)-O(1)	1.505(3)	C(11)-H(11)	0.9500
P(1)-C(7)	1.769(4)	C(12)-C(13)	1.364(7)
P(1)-C(16)	1.798(5)	C(12)-H(12)	0.9500
P(1)-C(10)	1.810(5)	C(13)-C(14)	1.370(7)
P(2)-O(2)	1.512(3)	C(13)-H(13)	0.9500
P(2)-C(8)	1.790(4)	C(14)-C(15)	1.364(7)
P(2)-C(28)	1.795(5)	C(14)-H(14)	0.9500
P(2)-C(22)	1.807(5)	C(15)-H(15)	0.9500
P(3)-C(9)	1.810(4)	C(16)-C(21)	1.389(6)
P(3)-C(40)	1.818(5)	C(16)-C(17)	1.393(6)
P(3)-C(34)	1.827(4)	C(17)-C(18)	1.354(7)
Cl(1)-Ni(2)	2.3311(12)	C(17)-H(17)	0.9500
B(1)-C(1)	1.647(6)	C(18)-C(19)	1.370(7)
B(1)-C(8)	1.660(7)	C(18)-H(18)	0.9500
B(1)-C(9)	1.675(7)	C(19)-C(20)	1.391(7)
B(1)-C(7)	1.680(7)	C(19)-H(19)	0.9500
Ni(2)-O(4)	1.980(3)	C(20)-C(21)	1.362(7)
Ni(2)-O(3)	2.006(3)	C(20)-H(20)	0.9500
Ni(2)-P(6)	2.3236(13)	C(21)-H(21)	0.9500
Ni(2)-Cl(2)	2.3916(11)	C(22)-C(23)	1.376(6)
Ni(2)-B(2)	3.912(4)	C(22)-C(27)	1.401(6)
P(4)-O(3)	1.503(3)	C(23)-C(24)	1.387(7)
P(4)-C(52)	1.770(4)	C(23)-H(23)	0.9500
P(4)-C(55)	1.805(5)	C(24)-C(25)	1.373(7)
P(4)-C(61)	1.808(5)	C(24)-H(24)	0.9500
P(5)-O(4)	1.511(3)	C(25)-C(26)	1.342(8)
P(5)-C(53)	1.774(4)	C(25)-H(25)	0.9500
P(5)-C(67)	1.807(4)	C(26)-C(27)	1.382(8)
P(5)-C(73)	1.807(4)	C(26)-H(26)	0.9500
P(6)-C(54)	1.810(4)	C(27)-H(27)	0.9500
P(6)-C(85)	1.825(5)	C(28)-C(33)	1.389(6)
P(6)-C(79)	1.832(4)	C(28)-C(29)	1.405(6)
B(2)-C(46)	1.646(6)	C(29)-C(30)	1.385(7)
B(2)-C(54)	1.668(6)	C(29)-H(29)	0.9500
B(2)-C(53)	1.686(6)	C(30)-C(31)	1.394(7)
B(2)-C(52)	1.692(7)	C(30)-H(30)	0.9500
C(1)-C(2)	1.391(7)	C(31)-C(32)	1.375(6)
C(1)-C(6)	1.397(7)	C(31)-H(31)	0.9500
C(2)-C(3)	1.397(7)	C(32)-C(33)	1.381(6)
C(2)-H(2)	0.9500	C(32)-H(32)	0.9500
C(3)-C(4)	1.370(9)	C(33)-H(33)	0.9500
C(3)-H(3)	0.9500	C(34)-C(35)	1.367(6)
C(4)-C(5)	1.359(9)	C(34)-C(39)	1.403(6)
C(4)-H(4)	0.9500	C(35)-C(36)	1.400(6)
C(5)-C(6)	1.399(7)	C(35)-H(35)	0.9500
C(5)-H(5)	0.9500	C(36)-C(37)	1.380(6)
C(6)-H(6)	0.9500	C(36)-H(36)	0.9500
C(7)-H(7A)	0.9900	C(37)-C(38)	1.380(7)
C(7)-H(7B)	0.9900	C(37)-H(37)	0.9500
C(8)-H(8A)	0.9900	C(38)-C(39)	1.372(6)

C(38)-H(38)	0.9500	C(70)-C(71)	1.367(7)
C(39)-H(39)	0.9500	C(70)-H(70)	0.9500
C(40)-C(45)	1.356(7)	C(71)-C(72)	1.382(6)
C(40)-C(41)	1.385(7)	C(71)-H(71)	0.9500
C(41)-C(42)	1.394(7)	C(72)-H(72)	0.9500
C(41)-H(41)	0.9500	C(73)-C(78)	1.398(5)
C(42)-C(43)	1.367(9)	C(73)-C(74)	1.399(5)
C(42)-H(42)	0.9500	C(74)-C(75)	1.375(6)
C(43)-C(44)	1.349(10)	C(74)-H(74)	0.9500
C(43)-H(43)	0.9500	C(75)-C(76)	1.384(6)
C(44)-C(45)	1.408(9)	C(75)-H(75)	0.9500
C(44)-H(44)	0.9500	C(76)-C(77)	1.379(6)
C(45)-H(45)	0.9500	C(76)-H(76)	0.9500
C(46)-C(47)	1.394(6)	C(77)-C(78)	1.373(6)
C(46)-C(51)	1.398(6)	C(77)-H(77)	0.9500
C(47)-C(48)	1.400(6)	C(78)-H(78)	0.9500
C(47)-H(47)	0.9500	C(79)-C(80)	1.391(5)
C(48)-C(49)	1.379(7)	C(79)-C(84)	1.399(6)
C(48)-H(48)	0.9500	C(80)-C(81)	1.393(6)
C(49)-C(50)	1.365(6)	C(80)-H(80)	0.9500
C(49)-H(49)	0.9500	C(81)-C(82)	1.382(6)
C(50)-C(51)	1.397(6)	C(81)-H(81)	0.9500
C(50)-H(50)	0.9500	C(82)-C(83)	1.383(6)
C(51)-H(51)	0.9500	C(82)-H(82)	0.9500
C(52)-H(52A)	0.9900	C(83)-C(84)	1.376(6)
C(52)-H(52B)	0.9900	C(83)-H(83)	0.9500
C(53)-H(53A)	0.9900	C(84)-H(84)	0.9500
C(53)-H(53B)	0.9900	C(85)-C(90)	1.322(6)
C(54)-H(54A)	0.9900	C(85)-C(86)	1.373(6)
C(54)-H(54B)	0.9900	C(86)-C(87)	1.373(8)
C(55)-C(60)	1.393(6)	C(86)-H(86)	0.9500
C(55)-C(56)	1.398(6)	C(87)-C(88)	1.329(8)
C(56)-C(57)	1.388(7)	C(87)-H(87)	0.9500
C(56)-H(56)	0.9500	C(88)-C(89)	1.345(9)
C(57)-C(58)	1.362(7)	C(88)-H(88)	0.9500
C(57)-H(57)	0.9500	C(89)-C(90)	1.387(8)
C(58)-C(59)	1.383(7)	C(89)-H(89)	0.9500
C(58)-H(58)	0.9500	C(90)-H(90)	0.9500
C(59)-C(60)	1.389(7)	C(91A)-Cl(3)	1.59(3)
C(59)-H(59)	0.9500	C(91A)-Cl(4)	1.788(16)
C(60)-H(60)	0.9500	C(91A)-H(91A)	0.9900
C(61)-C(62)	1.383(6)	C(91A)-H(91B)	0.9900
C(61)-C(66)	1.384(6)	C(91B)-Cl(4)	2.07(7)
C(62)-C(63)	1.375(7)	C(91B)-Cl(3)	2.26(7)
C(62)-H(62)	0.9500	C(91B)-H(91C)	0.9900
C(63)-C(64)	1.376(7)	C(91B)-H(91D)	0.9900
C(63)-H(63)	0.9500	Cl(4)-C(91A)#1	1.788(16)
C(64)-C(65)	1.340(7)	Cl(4)-C(91B)#1	2.07(7)
C(64)-H(64)	0.9500	C(92)-C(93)	1.355(12)
C(65)-C(66)	1.381(7)	C(92)-H(92A)	0.9800
C(65)-H(65)	0.9500	C(92)-H(92B)	0.9800
C(66)-H(66)	0.9500	C(92)-H(92C)	0.9800
C(67)-C(68)	1.395(6)	C(100)-C(105)	1.467(17)
C(67)-C(72)	1.400(6)	C(100)-C(101)	1.505(15)
C(68)-C(69)	1.386(7)	C(100)-H(100)	0.9500
C(68)-H(68)	0.9500	C(101)-C(102)	1.467(11)
C(69)-C(70)	1.378(7)	C(101)-H(101)	0.9500
C(69)-H(69)	0.9500	C(102)-C(103)	1.471(12)

C(102)-H(102)	0.9500	O(2)-Ni(1)-B(1)	68.07(11)
C(103)-C(104)	1.399(16)	O(1)-Ni(1)-B(1)	59.55(11)
C(103)-H(103)	0.9500	P(3)-Ni(1)-B(1)	50.09(9)
C(104)-C(105)	1.376(18)	Cl(1)-Ni(1)-B(1)	125.74(8)
C(104)-H(104)	0.9500	Cl(2)-Ni(1)-B(1)	142.40(8)
C(105)-H(105)	0.9500	O(1)-P(1)-C(7)	116.08(18)
C(106)-C(111)	1.04(4)	O(1)-P(1)-C(16)	109.21(19)
C(106)-C(107)	1.55(3)	C(7)-P(1)-C(16)	108.6(2)
C(106)-H(106)	0.9500	O(1)-P(1)-C(10)	110.80(19)
C(107)-C(108)	1.39(5)	C(7)-P(1)-C(10)	108.3(2)
C(107)-H(107)	0.9500	C(16)-P(1)-C(10)	103.0(2)
C(108)-C(109)	1.27(4)	O(2)-P(2)-C(8)	117.8(2)
C(108)-H(108)	0.9500	O(2)-P(2)-C(28)	107.74(19)
C(109)-C(110)	1.31(3)	C(8)-P(2)-C(28)	106.6(2)
C(109)-H(109)	0.9500	O(2)-P(2)-C(22)	108.27(19)
C(110)-C(111)	1.59(3)	C(8)-P(2)-C(22)	109.8(2)
C(110)-H(110)	0.9500	C(28)-P(2)-C(22)	105.8(2)
C(111)-C(112)	1.55(4)	C(9)-P(3)-C(40)	108.8(2)
C(112)-H(11A)	0.9802	C(9)-P(3)-C(34)	105.10(19)
C(112)-H(11B)	0.9802	C(40)-P(3)-C(34)	101.8(2)
C(112)-H(11C)	0.9802	C(9)-P(3)-Ni(1)	111.86(16)
C(113)-C(114)	1.72(4)	C(40)-P(3)-Ni(1)	112.25(14)
C(113)-H(11A)	0.9803	C(34)-P(3)-Ni(1)	116.20(15)
C(113)-H(11B)	0.9803	P(1)-O(1)-Ni(1)	148.84(18)
C(113)-H(11C)	0.9803	P(2)-O(2)-Ni(1)	136.93(19)
C(114)-C(115)	1.16(3)	Ni(2)-Cl(1)-Ni(1)	97.20(4)
C(114)-C(119)	1.69(3)	C(1)-B(1)-C(8)	103.5(3)
C(115)-C(116)	1.43(3)	C(1)-B(1)-C(9)	109.6(4)
C(115)-H(115)	0.9500	C(8)-B(1)-C(9)	115.0(4)
C(116)-C(117)	1.52(4)	C(1)-B(1)-C(7)	106.5(4)
C(116)-H(116)	0.9500	C(8)-B(1)-C(7)	109.7(4)
C(117)-C(118)	1.14(5)	C(9)-B(1)-C(7)	111.8(3)
C(117)-H(117)	0.9500	C(1)-B(1)-Ni(1)	167.4(3)
C(118)-C(119)	1.34(5)	C(8)-B(1)-Ni(1)	76.2(2)
C(118)-H(118)	0.9500	C(9)-B(1)-Ni(1)	60.4(2)
C(119)-H(119)	0.9500	C(7)-B(1)-Ni(1)	85.2(2)
C(93)-C(98)	1.147(15)	O(4)-Ni(2)-O(3)	88.71(11)
C(93)-C(94)	1.5008	O(4)-Ni(2)-P(6)	98.62(8)
C(94)-C(95)	1.388(17)	O(3)-Ni(2)-P(6)	99.80(8)
C(94)-H(94)	0.9500	O(4)-Ni(2)-Cl(1)	160.59(8)
C(95)-C(96)	1.86(3)	O(3)-Ni(2)-Cl(1)	89.98(9)
C(95)-H(95)	0.9500	P(6)-Ni(2)-Cl(1)	100.69(5)
C(96)-C(97)	0.827(17)	O(4)-Ni(2)-Cl(2)	90.03(8)
C(96)-H(96)	0.9500	O(3)-Ni(2)-Cl(2)	158.33(9)
C(97)-C(98)	1.650(15)	P(6)-Ni(2)-Cl(2)	101.78(4)
C(97)-H(97)	0.9500	Cl(1)-Ni(2)-Cl(2)	84.11(4)
C(98)-H(98)	0.9500	O(4)-Ni(2)-B(2)	68.64(10)
		O(3)-Ni(2)-B(2)	60.03(11)
O(2)-Ni(1)-O(1)	90.82(12)	P(6)-Ni(2)-B(2)	50.62(9)
O(2)-Ni(1)-P(3)	95.05(9)	Cl(1)-Ni(2)-B(2)	126.53(8)
O(1)-Ni(1)-P(3)	99.50(9)	Cl(2)-Ni(2)-B(2)	138.47(8)
O(2)-Ni(1)-Cl(1)	162.37(9)	O(3)-P(4)-C(52)	115.33(18)
O(1)-Ni(1)-Cl(1)	88.57(8)	O(3)-P(4)-C(55)	110.61(19)
P(3)-Ni(1)-Cl(1)	102.43(5)	C(52)-P(4)-C(55)	109.2(2)
O(2)-Ni(1)-Cl(2)	89.14(9)	O(3)-P(4)-C(61)	107.89(19)
O(1)-Ni(1)-Cl(2)	154.17(9)	C(52)-P(4)-C(61)	109.6(2)
P(3)-Ni(1)-Cl(2)	106.23(5)	C(55)-P(4)-C(61)	103.5(2)
Cl(1)-Ni(1)-Cl(2)	83.84(4)	O(4)-P(5)-C(53)	118.10(18)

O(4)-P(5)-C(67)	110.00(18)	P(3)-C(9)-H(9B)	107.3
C(53)-P(5)-C(67)	108.60(19)	H(9A)-C(9)-H(9B)	106.9
O(4)-P(5)-C(73)	106.89(17)	C(11)-C(10)-C(15)	117.2(5)
C(53)-P(5)-C(73)	106.44(19)	C(11)-C(10)-P(1)	121.0(4)
C(67)-P(5)-C(73)	106.1(2)	C(15)-C(10)-P(1)	121.7(4)
C(54)-P(6)-C(85)	105.14(19)	C(10)-C(11)-C(12)	121.5(5)
C(54)-P(6)-C(79)	104.76(19)	C(10)-C(11)-H(11)	119.2
C(85)-P(6)-C(79)	102.3(2)	C(12)-C(11)-H(11)	119.3
C(54)-P(6)-Ni(2)	111.82(15)	C(13)-C(12)-C(11)	120.8(5)
C(85)-P(6)-Ni(2)	115.09(14)	C(13)-C(12)-H(12)	119.5
C(79)-P(6)-Ni(2)	116.51(14)	C(11)-C(12)-H(12)	119.6
P(4)-O(3)-Ni(2)	146.79(18)	C(12)-C(13)-C(14)	119.1(5)
P(5)-O(4)-Ni(2)	136.77(16)	C(12)-C(13)-H(13)	120.5
Ni(1)-Cl(2)-Ni(2)	94.84(4)	C(14)-C(13)-H(13)	120.5
C(46)-B(2)-C(54)	108.7(4)	C(15)-C(14)-C(13)	120.3(5)
C(46)-B(2)-C(53)	103.5(3)	C(15)-C(14)-H(14)	119.9
C(54)-B(2)-C(53)	115.0(3)	C(13)-C(14)-H(14)	119.8
C(46)-B(2)-C(52)	107.6(3)	C(14)-C(15)-C(10)	121.1(5)
C(54)-B(2)-C(52)	111.5(4)	C(14)-C(15)-H(15)	119.5
C(53)-B(2)-C(52)	110.0(4)	C(10)-C(15)-H(15)	119.4
C(46)-B(2)-Ni(2)	166.7(3)	C(21)-C(16)-C(17)	118.6(5)
C(54)-B(2)-Ni(2)	61.23(18)	C(21)-C(16)-P(1)	119.8(4)
C(53)-B(2)-Ni(2)	75.40(19)	C(17)-C(16)-P(1)	121.6(4)
C(52)-B(2)-Ni(2)	85.0(2)	C(18)-C(17)-C(16)	121.8(5)
C(2)-C(1)-C(6)	115.5(5)	C(18)-C(17)-H(17)	119.1
C(2)-C(1)-B(1)	124.4(5)	C(16)-C(17)-H(17)	119.1
C(6)-C(1)-B(1)	120.0(5)	C(17)-C(18)-C(19)	119.2(5)
C(1)-C(2)-C(3)	121.4(6)	C(17)-C(18)-H(18)	120.5
C(1)-C(2)-H(2)	119.3	C(19)-C(18)-H(18)	120.4
C(3)-C(2)-H(2)	119.3	C(18)-C(19)-C(20)	120.2(5)
C(4)-C(3)-C(2)	121.6(7)	C(18)-C(19)-H(19)	119.9
C(4)-C(3)-H(3)	119.2	C(20)-C(19)-H(19)	119.9
C(2)-C(3)-H(3)	119.2	C(21)-C(20)-C(19)	120.5(5)
C(5)-C(4)-C(3)	118.6(6)	C(21)-C(20)-H(20)	119.7
C(5)-C(4)-H(4)	120.7	C(19)-C(20)-H(20)	119.8
C(3)-C(4)-H(4)	120.7	C(20)-C(21)-C(16)	119.7(5)
C(4)-C(5)-C(6)	120.3(7)	C(20)-C(21)-H(21)	120.1
C(4)-C(5)-H(5)	119.8	C(16)-C(21)-H(21)	120.1
C(6)-C(5)-H(5)	119.9	C(23)-C(22)-C(27)	117.4(5)
C(1)-C(6)-C(5)	122.7(6)	C(23)-C(22)-P(2)	119.6(4)
C(1)-C(6)-H(6)	118.6	C(27)-C(22)-P(2)	123.0(4)
C(5)-C(6)-H(6)	118.7	C(22)-C(23)-C(24)	121.9(5)
B(1)-C(7)-P(1)	119.1(3)	C(22)-C(23)-H(23)	119.0
B(1)-C(7)-H(7A)	107.5	C(24)-C(23)-H(23)	119.1
P(1)-C(7)-H(7A)	107.5	C(25)-C(24)-C(23)	119.1(6)
B(1)-C(7)-H(7B)	107.6	C(25)-C(24)-H(24)	120.5
P(1)-C(7)-H(7B)	107.5	C(23)-C(24)-H(24)	120.4
H(7A)-C(7)-H(7B)	107.0	C(26)-C(25)-C(24)	120.1(6)
B(1)-C(8)-P(2)	127.1(3)	C(26)-C(25)-H(25)	119.9
B(1)-C(8)-H(8A)	105.5	C(24)-C(25)-H(25)	120.0
P(2)-C(8)-H(8A)	105.5	C(25)-C(26)-C(27)	121.6(6)
B(1)-C(8)-H(8B)	105.5	C(25)-C(26)-H(26)	119.3
P(2)-C(8)-H(8B)	105.5	C(27)-C(26)-H(26)	119.1
H(8A)-C(8)-H(8B)	106.1	C(26)-C(27)-C(22)	119.9(5)
B(1)-C(9)-P(3)	120.1(3)	C(26)-C(27)-H(27)	120.1
B(1)-C(9)-H(9A)	107.3	C(22)-C(27)-H(27)	120.0
P(3)-C(9)-H(9A)	107.3	C(33)-C(28)-C(29)	117.7(4)
B(1)-C(9)-H(9B)	107.3	C(33)-C(28)-P(2)	120.5(3)

C(29)-C(28)-P(2)	121.7(4)	C(49)-C(48)-C(47)	120.4(4)
C(30)-C(29)-C(28)	120.5(5)	C(49)-C(48)-H(48)	119.8
C(30)-C(29)-H(29)	119.7	C(47)-C(48)-H(48)	119.8
C(28)-C(29)-H(29)	119.8	C(50)-C(49)-C(48)	119.2(4)
C(29)-C(30)-C(31)	120.7(5)	C(50)-C(49)-H(49)	120.4
C(29)-C(30)-H(30)	119.6	C(48)-C(49)-H(49)	120.4
C(31)-C(30)-H(30)	119.7	C(49)-C(50)-C(51)	119.9(5)
C(32)-C(31)-C(30)	118.7(5)	C(49)-C(50)-H(50)	120.0
C(32)-C(31)-H(31)	120.6	C(51)-C(50)-H(50)	120.1
C(30)-C(31)-H(31)	120.7	C(50)-C(51)-C(46)	123.1(4)
C(31)-C(32)-C(33)	120.9(5)	C(50)-C(51)-H(51)	118.5
C(31)-C(32)-H(32)	119.6	C(46)-C(51)-H(51)	118.4
C(33)-C(32)-H(32)	119.5	B(2)-C(52)-P(4)	118.5(3)
C(32)-C(33)-C(28)	121.4(4)	B(2)-C(52)-H(52A)	107.8
C(32)-C(33)-H(33)	119.3	P(4)-C(52)-H(52A)	107.7
C(28)-C(33)-H(33)	119.4	B(2)-C(52)-H(52B)	107.6
C(35)-C(34)-C(39)	118.9(4)	P(4)-C(52)-H(52B)	107.7
C(35)-C(34)-P(3)	121.0(3)	H(52A)-C(52)-H(52B)	107.1
C(39)-C(34)-P(3)	120.1(4)	B(2)-C(53)-P(5)	126.7(3)
C(34)-C(35)-C(36)	120.4(4)	B(2)-C(53)-H(53A)	105.6
C(34)-C(35)-H(35)	119.8	P(5)-C(53)-H(53A)	105.6
C(36)-C(35)-H(35)	119.9	B(2)-C(53)-H(53B)	105.7
C(37)-C(36)-C(35)	120.5(5)	P(5)-C(53)-H(53B)	105.6
C(37)-C(36)-H(36)	119.8	H(53A)-C(53)-H(53B)	106.1
C(35)-C(36)-H(36)	119.7	B(2)-C(54)-P(6)	121.0(3)
C(36)-C(37)-C(38)	119.0(4)	B(2)-C(54)-H(54A)	107.0
C(36)-C(37)-H(37)	120.5	P(6)-C(54)-H(54A)	107.1
C(38)-C(37)-H(37)	120.5	B(2)-C(54)-H(54B)	107.1
C(39)-C(38)-C(37)	120.8(5)	P(6)-C(54)-H(54B)	107.1
C(39)-C(38)-H(38)	119.6	H(54A)-C(54)-H(54B)	106.8
C(37)-C(38)-H(38)	119.6	C(60)-C(55)-C(56)	118.4(4)
C(38)-C(39)-C(34)	120.5(5)	C(60)-C(55)-P(4)	124.5(4)
C(38)-C(39)-H(39)	119.7	C(56)-C(55)-P(4)	117.1(4)
C(34)-C(39)-H(39)	119.8	C(57)-C(56)-C(55)	120.3(5)
C(45)-C(40)-C(41)	118.4(5)	C(57)-C(56)-H(56)	119.9
C(45)-C(40)-P(3)	123.5(5)	C(55)-C(56)-H(56)	119.8
C(41)-C(40)-P(3)	118.0(4)	C(58)-C(57)-C(56)	120.8(5)
C(40)-C(41)-C(42)	120.6(6)	C(58)-C(57)-H(57)	119.6
C(40)-C(41)-H(41)	119.7	C(56)-C(57)-H(57)	119.6
C(42)-C(41)-H(41)	119.7	C(57)-C(58)-C(59)	119.7(5)
C(43)-C(42)-C(41)	120.3(6)	C(57)-C(58)-H(58)	120.2
C(43)-C(42)-H(42)	119.8	C(59)-C(58)-H(58)	120.1
C(41)-C(42)-H(42)	119.9	C(58)-C(59)-C(60)	120.5(5)
C(44)-C(43)-C(42)	119.3(6)	C(58)-C(59)-H(59)	119.8
C(44)-C(43)-H(43)	120.3	C(60)-C(59)-H(59)	119.7
C(42)-C(43)-H(43)	120.3	C(59)-C(60)-C(55)	120.2(5)
C(43)-C(44)-C(45)	120.7(7)	C(59)-C(60)-H(60)	119.9
C(43)-C(44)-H(44)	119.7	C(55)-C(60)-H(60)	119.9
C(45)-C(44)-H(44)	119.6	C(62)-C(61)-C(66)	118.4(5)
C(40)-C(45)-C(44)	120.6(6)	C(62)-C(61)-P(4)	119.6(4)
C(40)-C(45)-H(45)	119.7	C(66)-C(61)-P(4)	121.9(4)
C(44)-C(45)-H(45)	119.7	C(63)-C(62)-C(61)	119.8(5)
C(47)-C(46)-C(51)	115.0(4)	C(63)-C(62)-H(62)	120.1
C(47)-C(46)-B(2)	121.5(4)	C(61)-C(62)-H(62)	120.1
C(51)-C(46)-B(2)	123.5(4)	C(62)-C(63)-C(64)	120.9(5)
C(46)-C(47)-C(48)	122.3(4)	C(62)-C(63)-H(63)	119.5
C(46)-C(47)-H(47)	118.9	C(64)-C(63)-H(63)	119.6
C(48)-C(47)-H(47)	118.9	C(65)-C(64)-C(63)	119.7(5)

C(65)-C(64)-H(64)	120.1	C(82)-C(83)-H(83)	119.6
C(63)-C(64)-H(64)	120.2	C(83)-C(84)-C(79)	120.6(4)
C(64)-C(65)-C(66)	120.6(5)	C(83)-C(84)-H(84)	119.7
C(64)-C(65)-H(65)	119.8	C(79)-C(84)-H(84)	119.7
C(66)-C(65)-H(65)	119.7	C(90)-C(85)-C(86)	116.2(5)
C(65)-C(66)-C(61)	120.7(5)	C(90)-C(85)-P(6)	123.7(4)
C(65)-C(66)-H(66)	119.7	C(86)-C(85)-P(6)	120.1(4)
C(61)-C(66)-H(66)	119.6	C(87)-C(86)-C(85)	121.4(6)
C(68)-C(67)-C(72)	119.3(4)	C(87)-C(86)-H(86)	119.3
C(68)-C(67)-P(5)	117.9(3)	C(85)-C(86)-H(86)	119.3
C(72)-C(67)-P(5)	122.8(3)	C(88)-C(87)-C(86)	121.4(6)
C(69)-C(68)-C(67)	119.0(5)	C(88)-C(87)-H(87)	119.3
C(69)-C(68)-H(68)	120.5	C(86)-C(87)-H(87)	119.3
C(67)-C(68)-H(68)	120.5	C(87)-C(88)-C(89)	117.9(6)
C(70)-C(69)-C(68)	121.0(5)	C(87)-C(88)-H(88)	121.2
C(70)-C(69)-H(69)	119.5	C(89)-C(88)-H(88)	120.9
C(68)-C(69)-H(69)	119.5	C(88)-C(89)-C(90)	120.6(6)
C(71)-C(70)-C(69)	120.4(5)	C(88)-C(89)-H(89)	119.8
C(71)-C(70)-H(70)	119.8	C(90)-C(89)-H(89)	119.6
C(69)-C(70)-H(70)	119.8	C(85)-C(90)-C(89)	122.5(6)
C(70)-C(71)-C(72)	119.8(5)	C(85)-C(90)-H(90)	118.7
C(70)-C(71)-H(71)	120.1	C(89)-C(90)-H(90)	118.8
C(72)-C(71)-H(71)	120.1	Cl(3)-C(91A)-Cl(4)	98.2(15)
C(71)-C(72)-C(67)	120.5(4)	Cl(3)-C(91A)-H(91A)	112.2
C(71)-C(72)-H(72)	119.8	Cl(4)-C(91A)-H(91A)	112.0
C(67)-C(72)-H(72)	119.7	Cl(3)-C(91A)-H(91B)	112.2
C(78)-C(73)-C(74)	118.2(4)	Cl(4)-C(91A)-H(91B)	112.1
C(78)-C(73)-P(5)	122.3(3)	H(91A)-C(91A)-H(91B)	109.8
C(74)-C(73)-P(5)	119.4(3)	Cl(4)-C(91B)-Cl(3)	72(3)
C(75)-C(74)-C(73)	120.6(4)	Cl(4)-C(91B)-H(91C)	110.0
C(75)-C(74)-H(74)	119.7	Cl(3)-C(91B)-H(91C)	110.7
C(73)-C(74)-H(74)	119.7	Cl(4)-C(91B)-H(91D)	123.8
C(74)-C(75)-C(76)	120.3(4)	Cl(3)-C(91B)-H(91D)	122.9
C(74)-C(75)-H(75)	119.8	H(91C)-C(91B)-H(91D)	111.5
C(76)-C(75)-H(75)	119.8	C(91A)-Cl(3)-C(91B)	90.2(13)
C(77)-C(76)-C(75)	119.7(4)	C(91A)#1-Cl(4)-C(91A)	180.0(17)
C(77)-C(76)-H(76)	120.1	C(91A)#1-Cl(4)-C(91B)	88.4(15)
C(75)-C(76)-H(76)	120.2	C(91A)-Cl(4)-C(91B)	91.6(15)
C(78)-C(77)-C(76)	120.4(4)	C(91A)#1-Cl(4)-C(91B)#1	91.6(15)
C(78)-C(77)-H(77)	119.8	C(91A)-Cl(4)-C(91B)#1	88.4(15)
C(76)-C(77)-H(77)	119.9	C(91B)-Cl(4)-C(91B)#1	180(5)
C(77)-C(78)-C(73)	120.7(4)	C(93)-C(92)-H(92A)	109.9
C(77)-C(78)-H(78)	119.6	C(93)-C(92)-H(92B)	109.4
C(73)-C(78)-H(78)	119.6	H(92A)-C(92)-H(92B)	109.5
C(80)-C(79)-C(84)	118.2(4)	C(93)-C(92)-H(92C)	109.1
C(80)-C(79)-P(6)	120.5(3)	H(92A)-C(92)-H(92C)	109.5
C(84)-C(79)-P(6)	121.2(3)	H(92B)-C(92)-H(92C)	109.5
C(79)-C(80)-C(81)	121.0(4)	C(105)-C(100)-C(101)	102.6(15)
C(79)-C(80)-H(80)	119.5	C(105)-C(100)-H(100)	128.8
C(81)-C(80)-H(80)	119.5	C(101)-C(100)-H(100)	128.6
C(82)-C(81)-C(80)	119.8(4)	C(102)-C(101)-C(100)	123.6(11)
C(82)-C(81)-H(81)	120.1	C(102)-C(101)-H(101)	118.2
C(80)-C(81)-H(81)	120.1	C(100)-C(101)-H(101)	118.3
C(81)-C(82)-C(83)	119.5(4)	C(101)-C(102)-C(103)	121.6(9)
C(81)-C(82)-H(82)	120.3	C(101)-C(102)-H(102)	119.4
C(83)-C(82)-H(82)	120.2	C(103)-C(102)-H(102)	119.0
C(84)-C(83)-C(82)	120.8(4)	C(104)-C(103)-C(102)	118.9(13)
C(84)-C(83)-H(83)	119.6	C(104)-C(103)-H(103)	120.8

C(102)-C(103)-H(103)	120.3	C(114)-C(115)-C(116)	117(3)
C(105)-C(104)-C(103)	112.8(19)	C(114)-C(115)-H(115)	121.3
C(105)-C(104)-H(104)	123.5	C(116)-C(115)-H(115)	122.0
C(103)-C(104)-H(104)	123.7	C(115)-C(116)-C(117)	132(2)
C(104)-C(105)-C(100)	140.5(17)	C(115)-C(116)-H(116)	114.0
C(104)-C(105)-H(105)	110.3	C(117)-C(116)-H(116)	114.2
C(100)-C(105)-H(105)	109.2	C(118)-C(117)-C(116)	106(4)
C(111)-C(106)-C(107)	128(3)	C(118)-C(117)-H(117)	127.5
C(111)-C(106)-H(106)	116.0	C(116)-C(117)-H(117)	126.3
C(107)-C(106)-H(106)	116.0	C(117)-C(118)-C(119)	133(7)
C(108)-C(107)-C(106)	120(2)	C(117)-C(118)-H(118)	113.2
C(108)-C(107)-H(107)	120.0	C(119)-C(118)-H(118)	114.0
C(106)-C(107)-H(107)	120.0	C(118)-C(119)-C(114)	117(3)
C(109)-C(108)-C(107)	115(3)	C(118)-C(119)-H(119)	121.4
C(109)-C(108)-H(108)	122.0	C(114)-C(119)-H(119)	121.3
C(107)-C(108)-H(108)	122.6	C(98)-C(93)-C(92)	142.7(17)
C(108)-C(109)-C(110)	120(3)	C(98)-C(93)-C(94)	104.0(10)
C(108)-C(109)-H(109)	120.3	C(92)-C(93)-C(94)	112.7(9)
C(110)-C(109)-H(109)	119.5	C(95)-C(94)-C(93)	128.2(14)
C(109)-C(110)-C(111)	128(2)	C(95)-C(94)-H(94)	116.3
C(109)-C(110)-H(110)	116.2	C(93)-C(94)-H(94)	115.5
C(111)-C(110)-H(110)	116.2	C(94)-C(95)-C(96)	95.8(16)
C(106)-C(111)-C(112)	134(3)	C(94)-C(95)-H(95)	128.7
C(106)-C(111)-C(110)	109(3)	C(96)-C(95)-H(95)	135.5
C(112)-C(111)-C(110)	115(2)	C(97)-C(96)-C(95)	156.3(19)
C(114)-C(113)-H(11A)	109.8	C(97)-C(96)-H(96)	102.0
C(114)-C(113)-H(11B)	109.2	C(95)-C(96)-H(96)	101.6
H(11A)-C(113)-H(11B)	109.5	C(96)-C(97)-C(98)	87.9(13)
C(114)-C(113)-H(11C)	109.5	C(96)-C(97)-H(97)	137.7
H(11A)-C(113)-H(11C)	109.4	C(98)-C(97)-H(97)	134.4
H(11B)-C(113)-H(11C)	109.4	C(93)-C(98)-C(97)	146.9(14)
C(115)-C(114)-C(119)	115(3)	C(93)-C(98)-H(98)	107.8
C(115)-C(114)-C(113)	120(3)	C(97)-C(98)-H(98)	105.3
C(119)-C(114)-C(113)	126(2)		

Symmetry transformations used to generate equivalent atoms:
#1 -x,-y+2,-z

Table 41. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for 8B · C_6H_6· 2 C_7H_8 · $CH_2Cl_{1.5}$. The anisotropic displacement factor exponent takes the form: $-2\pi^2[\ h^2a^{*2}U^{11} + ... + 2\ h\ k\ a^*\ b^*\ U^{12}]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Ni(1)	18(1)	24(1)	17(1)	-2(1)	7(1)	-2(1)
P(1)	21(1)	30(1)	21(1)	-4(1)	12(1)	-3(1)
P(2)	20(1)	30(1)	24(1)	-8(1)	11(1)	-5(1)
P(3)	24(1)	26(1)	19(1)	0(1)	9(1)	2(1)
O(1)	19(2)	28(2)	25(2)	-3(1)	13(1)	-1(1)
O(2)	20(2)	27(2)	21(2)	-6(1)	6(1)	-4(1)
Cl(1)	20(1)	33(1)	21(1)	-8(1)	9(1)	-5(1)
B(1)	19(3)	36(4)	19(3)	-7(2)	9(2)	0(2)
Ni(2)	17(1)	20(1)	18(1)	-3(1)	7(1)	-1(1)
P(4)	23(1)	19(1)	23(1)	-6(1)	11(1)	-2(1)
P(5)	19(1)	17(1)	17(1)	-1(1)	7(1)	-1(1)
P(6)	21(1)	19(1)	17(1)	-2(1)	8(1)	-1(1)
O(3)	22(2)	23(2)	23(2)	-3(1)	8(1)	-1(1)
O(4)	15(2)	23(2)	18(2)	0(1)	6(1)	0(1)
Cl(2)	17(1)	30(1)	19(1)	-7(1)	8(1)	-4(1)
B(2)	17(2)	24(3)	20(3)	-2(2)	8(2)	0(2)
C(1)	24(3)	50(4)	29(3)	-11(3)	10(2)	4(2)
C(2)	32(3)	50(4)	57(4)	-12(3)	-4(3)	12(3)
C(3)	47(4)	69(5)	63(4)	-20(4)	-9(3)	28(4)
C(4)	25(3)	118(7)	48(4)	-37(4)	0(3)	27(4)
C(5)	26(3)	134(7)	40(4)	-10(4)	5(3)	-1(4)
C(6)	24(3)	92(6)	40(3)	-1(3)	5(3)	-2(3)
C(7)	21(2)	34(3)	26(3)	-4(2)	10(2)	0(2)
C(8)	20(2)	36(3)	21(2)	2(2)	8(2)	-1(2)
C(9)	31(3)	36(3)	17(2)	-3(2)	9(2)	7(2)
C(10)	25(3)	37(3)	21(2)	-3(2)	10(2)	1(2)
C(11)	37(3)	44(4)	41(3)	-13(3)	18(3)	-4(3)
C(12)	47(3)	47(4)	67(4)	-26(3)	32(3)	-13(3)
C(13)	53(4)	48(4)	58(4)	-23(3)	29(3)	1(3)
C(14)	27(3)	80(5)	59(4)	-33(4)	19(3)	-1(3)
C(15)	30(3)	65(4)	46(3)	-27(3)	19(2)	-6(3)
C(16)	25(3)	35(3)	23(3)	-2(2)	12(2)	-1(2)
C(17)	26(3)	54(4)	35(3)	11(3)	11(2)	-6(2)
C(18)	37(3)	66(5)	51(4)	16(3)	18(3)	-8(3)
C(19)	58(4)	68(5)	63(4)	34(4)	34(3)	0(3)
C(20)	40(3)	84(5)	52(4)	34(3)	25(3)	13(3)
C(21)	35(3)	50(4)	46(4)	18(3)	25(3)	8(3)
C(22)	25(3)	23(3)	41(3)	-5(2)	21(2)	2(2)
C(23)	44(3)	31(3)	38(3)	-5(2)	28(3)	-9(2)
C(24)	67(4)	35(4)	56(4)	7(3)	40(3)	3(3)
C(25)	56(4)	32(4)	120(6)	16(4)	58(4)	2(3)
C(26)	41(4)	48(5)	132(7)	8(4)	34(4)	-14(3)
C(27)	33(3)	40(4)	87(5)	12(3)	18(3)	-7(3)
C(28)	25(3)	36(3)	30(3)	-15(2)	9(2)	-5(2)
C(29)	27(3)	105(6)	54(4)	-45(4)	19(3)	-18(3)
C(30)	34(4)	141(7)	54(4)	-62(4)	13(3)	-18(4)
C(31)	50(4)	90(5)	37(3)	-30(3)	21(3)	9(3)
C(32)	32(3)	41(3)	30(3)	-4(2)	16(2)	8(2)
C(33)	25(3)	27(3)	28(3)	-2(2)	12(2)	2(2)
C(34)	19(2)	30(3)	17(2)	3(2)	7(2)	1(2)
C(35)	21(2)	30(3)	24(3)	0(2)	7(2)	-4(2)
C(36)	30(3)	30(3)	24(3)	-3(2)	14(2)	-5(2)
C(37)	29(3)	46(4)	18(2)	1(2)	8(2)	-8(2)

C(38)	32(3)	53(4)	26(3)	12(3)	7(2)	13(3)
C(39)	33(3)	46(4)	24(3)	8(3)	13(2)	11(2)
C(40)	38(3)	24(3)	26(3)	5(2)	8(2)	5(2)
C(41)	55(4)	37(4)	46(4)	-11(3)	24(3)	-15(3)
C(42)	72(4)	47(4)	45(4)	12(3)	9(3)	-26(4)
C(43)	83(5)	23(4)	80(5)	5(4)	-8(4)	-11(4)
C(44)	85(6)	37(5)	183(9)	-51(5)	50(6)	-2(4)
C(45)	54(4)	41(4)	106(5)	-27(4)	43(4)	-6(3)
C(46)	19(2)	30(3)	10(2)	-1(2)	7(2)	1(2)
C(47)	26(3)	32(3)	19(2)	6(2)	4(2)	-5(2)
C(48)	24(3)	45(4)	33(3)	1(3)	6(2)	-8(2)
C(49)	21(3)	47(4)	23(3)	3(2)	2(2)	6(2)
C(50)	32(3)	35(3)	35(3)	0(2)	10(2)	9(2)
C(51)	26(3)	27(3)	27(3)	-9(2)	5(2)	2(2)
C(52)	20(2)	28(3)	18(2)	-9(2)	8(2)	-5(2)
C(53)	20(2)	14(2)	23(2)	-3(2)	10(2)	-1(2)
C(54)	20(2)	23(3)	14(2)	1(2)	7(2)	-1(2)
C(55)	35(3)	20(3)	26(3)	-10(2)	16(2)	-2(2)
C(56)	39(3)	48(4)	35(3)	-18(3)	19(3)	-14(3)
C(57)	58(4)	73(5)	54(4)	-29(3)	45(3)	-22(3)
C(58)	87(5)	40(4)	52(4)	-1(3)	57(4)	1(3)
C(59)	64(4)	51(4)	35(3)	14(3)	30(3)	22(3)
C(60)	36(3)	45(4)	35(3)	-1(3)	22(2)	6(3)
C(61)	26(2)	22(3)	30(3)	-6(2)	16(2)	-1(2)
C(62)	61(4)	25(3)	41(3)	-9(3)	1(3)	5(3)
C(63)	100(5)	33(4)	47(4)	1(3)	7(4)	21(4)
C(64)	64(4)	19(3)	65(4)	-11(3)	42(3)	-6(3)
C(65)	31(3)	34(4)	81(4)	-22(3)	15(3)	-7(3)
C(66)	33(3)	28(3)	64(4)	-15(3)	12(3)	-1(2)
C(67)	29(2)	15(2)	14(2)	1(2)	11(2)	-1(2)
C(68)	32(3)	22(3)	53(3)	7(3)	15(3)	2(2)
C(69)	53(4)	20(3)	91(5)	9(3)	29(3)	11(3)
C(70)	62(4)	18(3)	56(4)	-1(3)	27(3)	-8(3)
C(71)	44(3)	27(3)	39(3)	-7(3)	19(3)	-15(3)
C(72)	29(3)	23(3)	36(3)	2(2)	12(2)	-2(2)
C(73)	25(2)	14(2)	17(2)	4(2)	9(2)	1(2)
C(74)	20(2)	24(3)	19(2)	1(2)	8(2)	-1(2)
C(75)	32(3)	30(3)	19(2)	-7(2)	10(2)	-8(2)
C(76)	40(3)	23(3)	31(3)	-2(2)	22(2)	0(2)
C(77)	25(2)	31(3)	29(3)	-1(2)	16(2)	2(2)
C(78)	26(2)	28(3)	17(2)	-3(2)	9(2)	-3(2)
C(79)	16(2)	21(3)	15(2)	-4(2)	7(2)	-6(2)
C(80)	18(2)	14(2)	22(2)	-3(2)	4(2)	0(2)
C(81)	22(2)	20(3)	17(2)	-3(2)	9(2)	-5(2)
C(82)	19(2)	21(3)	22(2)	-4(2)	7(2)	2(2)
C(83)	25(2)	26(3)	22(3)	1(2)	6(2)	3(2)
C(84)	29(3)	22(3)	15(2)	1(2)	9(2)	1(2)
C(85)	22(2)	23(3)	24(3)	4(2)	8(2)	-1(2)
C(86)	56(4)	40(4)	68(4)	-28(3)	45(3)	-24(3)
C(87)	63(4)	26(4)	123(6)	-11(4)	64(4)	-13(3)
C(88)	37(3)	85(6)	73(5)	54(4)	18(4)	-7(3)
C(89)	108(6)	232(11)	28(4)	-3(5)	29(4)	-113(7)
C(90)	98(5)	145(8)	30(3)	-30(4)	40(4)	-88(5)
C(91A)	480(40)	370(30)	70(14)	8(16)	-36(18)	350(30)
C(91B)	89(18)	490(60)	2000(200)	870(100)	-540(60)	-230(30)
Cl(3)	525(15)	650(20)	720(20)	-51(16)	221(16)	107(15)
Cl(4)	650(20)	560(20)	284(12)	-25(13)	110(13)	320(20)
C(92)	181(11)	190(15)	206(13)	-33(11)	-126(10)	12(9)

C(100)	0(4)	215(17)	288(19)	-24(15)	-8(7)	-11(6)
C(101)	18(4)	214(12)	70(6)	23(7)	3(4)	-4(5)
C(102)	24(3)	126(8)	91(6)	-24(6)	15(4)	11(4)
C(103)	20(4)	119(9)	212(13)	-25(9)	25(5)	0(5)
C(104)	31(5)	195(17)	330(20)	116(17)	6(8)	-30(7)
C(105)	21(4)	96(10)	310(20)	-49(13)	29(9)	-11(5)
C(106)	94(18)	72(18)	59(17)	1(14)	32(15)	8(14)
C(107)	79(15)	160(30)	92(17)	10(15)	50(13)	48(14)
C(108)	80(30)	90(20)	130(30)	-33(19)	40(30)	-11(18)
C(109)	83(18)	73(16)	58(14)	-11(13)	11(13)	7(13)
C(110)	38(10)	53(11)	65(14)	-17(10)	38(10)	-18(8)
C(111)	30(12)	88(17)	54(17)	-19(12)	23(12)	5(11)
C(112)	100(20)	91(19)	58(17)	-59(15)	32(14)	-22(15)
C(113)	69(16)	64(13)	92(17)	18(14)	-4(15)	3(10)
C(114)	100(20)	38(9)	69(15)	13(9)	36(17)	-13(11)
C(115)	129(17)	117(15)	67(12)	34(10)	35(12)	12(13)
C(116)	57(11)	140(20)	131(18)	43(15)	59(12)	21(11)
C(117)	112(18)	107(17)	200(30)	23(18)	19(18)	-55(15)
C(118)	340(60)	280(40)	430(60)	-10(40)	180(50)	-220(40)
C(119)	960(140)	62(16)	78(18)	29(12)	200(50)	110(40)
C(93)	201(15)	183(14)	234(17)	121(14)	137(14)	68(12)
C(94)	210(20)	104(18)	480(40)	20(20)	80(20)	94(16)
C(95)	350(20)	154(15)	630(40)	-190(20)	-190(20)	164(16)
C(96)	1010(30)	530(20)	408(12)	246(13)	685(17)	306(19)
C(97)	418(16)	280(14)	266(11)	197(10)	360(13)	181(12)
C(98)	207(13)	159(13)	135(10)	16(10)	31(10)	-35(9)

Table 42. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for 8B · C_6H_6· 2 C_7H_8 · $CH_2Cl_{1.5}$.

	x	y	z	U(eq)
H(2)	791	8311	-625	63
H(3)	-198	8587	-1045	83
H(4)	-898	7508	-1024	82
H(5)	-604	6150	-562	83
H(6)	382	5858	-138	65
H(7A)	1347	5532	379	32
H(7B)	1107	6464	542	32
H(8A)	1589	6436	-628	31
H(8B)	1196	5645	-526	31
H(9A)	1848	7991	421	34
H(9B)	1559	8308	-112	34
H(11)	2875	7774	1431	48
H(12)	2856	9117	1857	61
H(13)	2032	9497	2001	61
H(14)	1204	8548	1683	65
H(15)	1206	7230	1236	54
H(17)	1189	5334	1199	47
H(18)	1181	4201	1735	61
H(19)	2047	3456	2199	71
H(20)	2926	3908	2145	67
H(21)	2939	5077	1620	49
H(23)	2769	4347	662	41
H(24)	2647	3033	1079	57
H(25)	1812	2093	762	74
H(26)	1096	2507	66	88
H(27)	1204	3810	-361	66
H(29)	1276	4376	-1054	73
H(30)	1296	3726	-1740	93
H(31)	2162	3736	-1880	69
H(32)	3010	4340	-1308	39
H(33)	3009	4900	-605	32
H(35)	2944	6754	-526	31
H(36)	2723	6681	-1333	32
H(37)	1986	7643	-1847	38
H(38)	1519	8754	-1546	46
H(39)	1739	8839	-750	41
H(41)	3449	8802	-32	53
H(42)	3912	10282	198	70
H(43)	3546	11394	572	88
H(44)	2778	10979	776	123
H(45)	2315	9488	555	76
H(47)	7186	8577	2275	32
H(48)	8129	8226	2797	42
H(49)	8376	6673	3083	39
H(50)	7700	5449	2789	41
H(51)	6762	5795	2260	33
H(52A)	6193	9069	1781	26
H(52B)	6278	8778	2301	26
H(53A)	6213	6728	1259	22
H(53B)	6609	7657	1368	22
H(54A)	5567	7054	2168	23
H(54B)	5952	6179	2122	23

H(56)	4252	8651	1950	47
H(57)	3956	8193	2548	65
H(58)	4634	7908	3293	61
H(59)	5627	8054	3447	56
H(60)	5939	8514	2855	43
H(62)	4486	10346	1291	58
H(63)	4404	12003	1291	79
H(64)	5104	12923	1854	53
H(65)	5898	12198	2404	61
H(66)	6005	10544	2409	53
H(68)	5015	9610	559	43
H(69)	5183	11261	585	65
H(70)	6124	11859	821	53
H(71)	6917	10831	1092	43
H(72)	6769	9182	1088	36
H(74)	5086	7196	-108	25
H(75)	5318	6496	-694	32
H(76)	6291	6343	-607	35
H(77)	7028	6967	53	32
H(78)	6807	7630	651	28
H(80)	5133	5976	557	23
H(81)	5592	4902	229	24
H(82)	6116	3605	669	25
H(83)	6170	3386	1431	30
H(84)	5760	4493	1772	26
H(86)	4310	4682	1183	58
H(87)	3838	3697	1521	75
H(88)	3919	3936	2274	79
H(89)	4485	5192	2690	146
H(90)	4963	6180	2351	104
H(91A)	448	9468	776	421
H(91B)	577	8724	426	421
H(91C)	632	11142	-309	1365
H(91D)	699	10033	-470	1365
H(92A)	2314	996	9434	378
H(92B)	1713	1089	9508	378
H(92C)	2004	2019	9385	378
H(100)	10021	2313	9327	224
H(101)	9994	4128	9417	126
H(102)	9982	5178	8808	99
H(103)	9984	4573	8077	148
H(104)	10029	2867	7980	245
H(105)	10029	1970	8575	185
H(106)	2489	1322	1469	89
H(107)	1440	1218	1283	127
H(108)	1080	1218	1893	117
H(109)	1750	1318	2627	91
H(110)	2686	1372	2755	56
H(11A)	3485	690	2384	121
H(11B)	3550	1814	2495	121
H(11C)	3513	1429	1998	121
H(11A)	1719	1340	2353	128
H(11B)	1519	1047	1814	128
H(11C)	1605	2153	1963	128
H(115)	2752	1743	2747	126
H(116)	3705	1748	2796	125
H(117)	4056	1508	2153	180
H(118)	3391	965	1554	402

H(119)	2440	996	1385	441
H(94)	987	494	9037	336
H(95)	323	-29	8262	586
H(96)	847	569	7689	629
H(97)	1525	917	7701	304
H(98)	2002	1605	8552	213

Figure 8. Fully-labeled displacement ellipsoid (50%) representation of [κ^2-PhB($CH_2P^iPr_2)_3$]Ni(dbabh) (**11**) (hydrogens omitted for clarity).

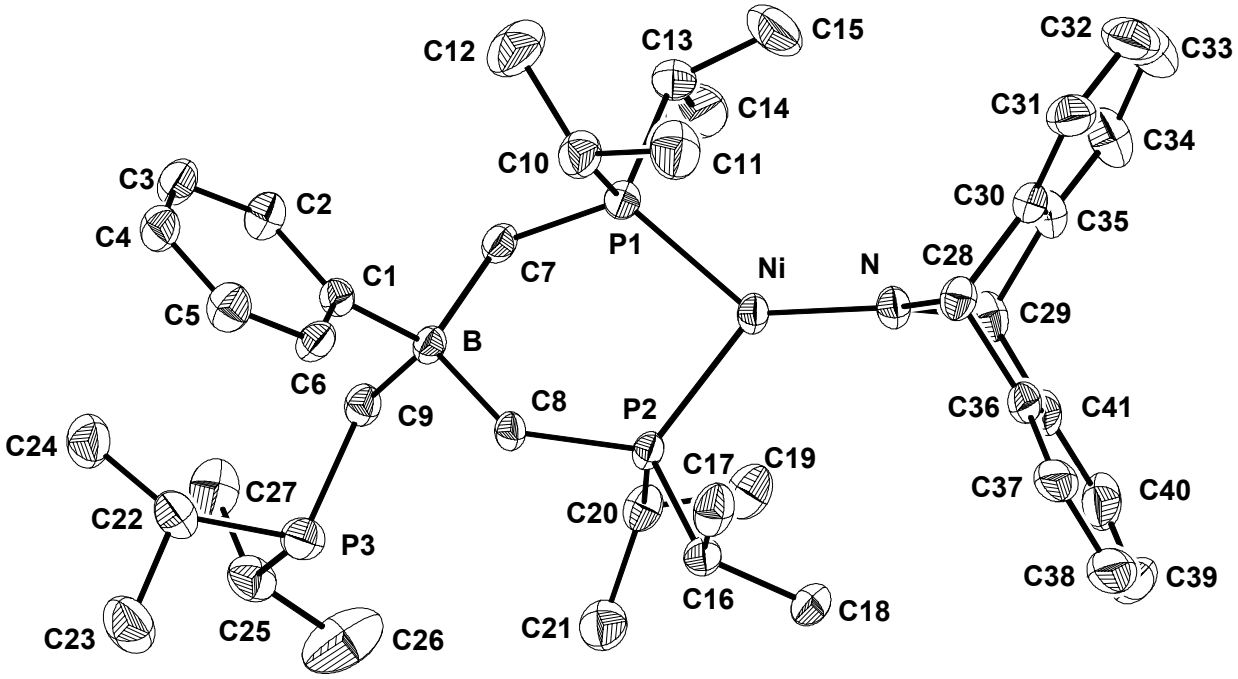


Table 43. Crystal data and structure refinement for 11.

Empirical formula	$C_{41}H_{63}BNNiP_3$	
Moiety formula	$C_{41}H_{63}BNNiP_3$	
Formula weight	732.35	
Crystal habit	block	
Crystal color	black	
Crystal size	0.33 x 0.30 x 0.23 mm^3	
Data Collection		
Type of diffractometer	CCD area detector	
Wavelength	0.71073 Å	
Temperature	100(2) K	
Unit cell dimensions	a = 12.0312(10) Å	α = 90°
	b = 26.359(2) Å	β = 99.150(2)°
	c = 12.9206(11) Å	γ = 90°
Volume	4045.4(6) $Å^3$	
Z	4	
Crystal system	Monoclinic	
Space group	$P2_1/n$	
Density (calculated)	1.202 g/cm^3	
F(000)	1576	
θ range for data collection	1.77 to 29.78°	
Completeness to θ = 29.78°	90.9%	
Index ranges	$-15 \le h \le 16$, $-36 \le k \le 36$, $-17 \le l \le 16$	
Reflections collected	48983	
Independent reflections	10516 [R(int) = 0.0685]	
Absorption coefficient	0.627 mm^{-1}	
Absorption correction	None	
Structure solution and refinement		
Structure solution program	SHELXS-97 (Sheldrick, 1990)	
Primary solution method	Direct methods	
Secondary solution method	Difference Fourier map	
Hydrogen placement	Calculated positions	
Structure refinement program	SHELXL-97 (Sheldrick, 1997)	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	10516 / 0 / 436	
Goodness-of-fit on F^2	1.577	
Final R indices [$I>2\sigma(I)$]	R1 = 0.0513, wR2 = 0.0943	
R indices (all data)	R1 = 0.0940, wR2 = 0.1015	
Type of weighting scheme used	calc	
Weighting scheme used	calc $w=1/[\sigma^2 (Fo^2)+(0.02P)^2]$ where $P=(Fo^2+2Fc^2)/3$	
Max shift/error	0.001	
Average shift/error	0.000	
Largest diff. peak and hole	1.084 and -0.512 $e \cdot Å^{-3}$	

Table 44. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$ x 10^3) for 11. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
Ni	6864(1)	1391(1)	4337(1)	22(1)
P(1)	7118(1)	1011(1)	2923(1)	25(1)
P(2)	5080(1)	1411(1)	3899(1)	21(1)
P(3)	2317(1)	647(1)	1598(1)	30(1)
N	7710(2)	1646(1)	5441(1)	24(1)
B	4780(2)	905(1)	1787(2)	21(1)
C(1)	4758(2)	1091(1)	567(2)	22(1)
C(2)	5043(2)	761(1)	-193(2)	30(1)
C(3)	4911(2)	879(1)	-1255(2)	34(1)
C(4)	4494(2)	1346(1)	-1598(2)	32(1)
C(5)	4220(2)	1689(1)	-888(2)	33(1)
C(6)	4343(2)	1563(1)	174(2)	28(1)
C(7)	6005(2)	618(1)	2251(2)	24(1)
C(8)	4525(2)	1395(1)	2522(2)	20(1)
C(9)	3796(2)	456(1)	1761(2)	25(1)
C(10)	7400(2)	1490(1)	1957(2)	34(1)
C(11)	8035(2)	1954(1)	2471(2)	47(1)
C(12)	7971(3)	1273(1)	1081(2)	56(1)
C(13)	8388(2)	602(1)	3239(2)	40(1)
C(14)	8141(3)	163(1)	3930(2)	55(1)
C(15)	9423(2)	902(1)	3750(3)	65(1)
C(16)	4539(2)	2011(1)	4381(2)	27(1)
C(17)	5106(2)	2465(1)	3937(2)	34(1)
C(18)	4684(2)	2049(1)	5578(2)	34(1)
C(19)	5107(2)	717(1)	5574(2)	38(1)
C(20)	4433(2)	875(1)	4512(2)	28(1)
C(21)	3185(2)	956(1)	4557(2)	39(1)
C(22)	1897(2)	800(1)	178(2)	34(1)
C(23)	706(2)	1018(1)	18(2)	51(1)
C(24)	2013(2)	384(1)	-629(2)	41(1)
C(25)	1568(2)	32(1)	1767(2)	35(1)
C(26)	1479(3)	-19(1)	2924(3)	73(1)
C(27)	2081(2)	-447(1)	1418(2)	44(1)
C(28)	8235(2)	2163(1)	5609(2)	25(1)
C(29)	8099(2)	1464(1)	6533(2)	29(1)
C(30)	9441(2)	2002(1)	6017(2)	26(1)
C(31)	10477(2)	2190(1)	5892(2)	36(1)
C(32)	11427(2)	1919(1)	6350(2)	49(1)
C(33)	11347(3)	1491(1)	6917(3)	52(1)
C(34)	10306(2)	1303(1)	7053(2)	43(1)
C(35)	9353(2)	1562(1)	6597(2)	29(1)
C(36)	7679(2)	2330(1)	6538(2)	27(1)
C(37)	7233(2)	2784(1)	6801(2)	37(1)
C(38)	6720(2)	2792(1)	7696(2)	50(1)
C(39)	6668(2)	2370(1)	8287(2)	54(1)
C(40)	7111(2)	1903(1)	8015(2)	44(1)
C(41)	7612(2)	1890(1)	7130(2)	30(1)

Table 45. Selected bond lengths [Å] and angles [°] for 11.

Ni-N	1.7480(18)
Ni-P(2)	2.1317(7)
Ni-P(1)	2.1475(7)
N-Ni-P(2)	129.65(7)
N-Ni-P(1)	136.86(7)
P(2)-Ni-P(1)	93.38(3)

Table 46. Bond lengths [Å] and angles [°] for 11.

Ni-N	1.7480(18)	C(17)-H(17A)	0.9800
Ni-P(2)	2.1317(7)	C(17)-H(17B)	0.9800
Ni-P(1)	2.1475(7)	C(17)-H(17C)	0.9800
P(1)-C(7)	1.802(2)	C(18)-H(18A)	0.9800
P(1)-C(10)	1.844(3)	C(18)-H(18B)	0.9800
P(1)-C(13)	1.861(3)	C(18)-H(18C)	0.9800
P(2)-C(8)	1.798(2)	C(19)-C(20)	1.536(3)
P(2)-C(20)	1.851(2)	C(19)-H(19A)	0.9800
P(2)-C(16)	1.856(2)	C(19)-H(19B)	0.9800
P(3)-C(9)	1.829(2)	C(19)-H(19C)	0.9800
P(3)-C(22)	1.867(3)	C(20)-C(21)	1.527(3)
P(3)-C(25)	1.883(3)	C(20)-H(20)	1.0000
N-C(29)	1.493(3)	C(21)-H(21A)	0.9800
N-C(28)	1.504(3)	C(21)-H(21B)	0.9800
B-C(1)	1.647(3)	C(21)-H(21C)	0.9800
B-C(8)	1.661(3)	C(22)-C(23)	1.527(4)
B-C(9)	1.670(3)	C(22)-C(24)	1.534(3)
B-C(7)	1.680(3)	C(22)-H(22)	1.0000
C(1)-C(2)	1.395(3)	C(23)-H(23A)	0.9800
C(1)-C(6)	1.405(3)	C(23)-H(23B)	0.9800
C(2)-C(3)	1.391(3)	C(23)-H(23C)	0.9800
C(2)-H(2)	0.9500	C(24)-H(24A)	0.9800
C(3)-C(4)	1.376(3)	C(24)-H(24B)	0.9800
C(3)-H(3)	0.9500	C(24)-H(24C)	0.9800
C(4)-C(5)	1.365(3)	C(25)-C(27)	1.506(4)
C(4)-H(4)	0.9500	C(25)-C(26)	1.522(4)
C(5)-C(6)	1.396(3)	C(25)-H(25)	1.0000
C(5)-H(5)	0.9500	C(26)-H(26A)	0.9800
C(6)-H(6)	0.9500	C(26)-H(26B)	0.9800
C(7)-H(7A)	0.9900	C(26)-H(26C)	0.9800
C(7)-H(7B)	0.9900	C(27)-H(27A)	0.9800
C(8)-H(8A)	0.9900	C(27)-H(27B)	0.9800
C(8)-H(8B)	0.9900	C(27)-H(27C)	0.9800
C(9)-H(9A)	0.9900	C(28)-C(30)	1.523(3)
C(9)-H(9B)	0.9900	C(28)-C(36)	1.529(3)
C(10)-C(12)	1.525(4)	C(28)-H(28)	1.0000
C(10)-C(11)	1.538(3)	C(29)-C(35)	1.520(3)
C(10)-H(10)	1.0000	C(29)-C(41)	1.531(3)
C(11)-H(11A)	0.9800	C(29)-H(29)	1.0000
C(11)-H(11B)	0.9800	C(30)-C(31)	1.374(3)
C(11)-H(11C)	0.9800	C(30)-C(35)	1.392(3)
C(12)-H(12A)	0.9800	C(31)-C(32)	1.397(4)
C(12)-H(12B)	0.9800	C(31)-H(31)	0.9500
C(12)-H(12C)	0.9800	C(32)-C(33)	1.357(4)
C(13)-C(14)	1.518(4)	C(32)-H(32)	0.9500
C(13)-C(15)	1.533(4)	C(33)-C(34)	1.385(4)
C(13)-H(13)	1.0000	C(33)-H(33)	0.9500
C(14)-H(14A)	0.9800	C(34)-C(35)	1.384(3)
C(14)-H(14B)	0.9800	C(34)-H(34)	0.9500
C(14)-H(14C)	0.9800	C(36)-C(37)	1.376(3)
C(15)-H(15A)	0.9800	C(36)-C(41)	1.400(3)
C(15)-H(15B)	0.9800	C(37)-C(38)	1.395(4)
C(15)-H(15C)	0.9800	C(37)-H(37)	0.9500
C(16)-C(18)	1.532(3)	C(38)-C(39)	1.357(4)
C(16)-C(17)	1.532(3)	C(38)-H(38)	0.9500
C(16)-H(16)	1.0000	C(39)-C(40)	1.406(4)

C(39)-H(39)	0.9500
C(40)-C(41)	1.375(3)
C(40)-H(40)	0.9500
N-Ni-P(2)	129.65(7)
N-Ni-P(1)	136.86(7)
P(2)-Ni-P(1)	93.38(3)
C(7)-P(1)-C(10)	105.60(11)
C(7)-P(1)-C(13)	107.06(12)
C(10)-P(1)-C(13)	108.18(13)
C(7)-P(1)-Ni	118.87(8)
C(10)-P(1)-Ni	108.87(8)
C(13)-P(1)-Ni	107.85(9)
C(8)-P(2)-C(20)	106.89(11)
C(8)-P(2)-C(16)	104.90(10)
C(20)-P(2)-C(16)	108.24(11)
C(8)-P(2)-Ni	117.50(8)
C(20)-P(2)-Ni	110.00(8)
C(16)-P(2)-Ni	108.89(8)
C(9)-P(3)-C(22)	106.20(11)
C(9)-P(3)-C(25)	103.00(11)
C(22)-P(3)-C(25)	103.92(12)
C(29)-N-C(28)	95.29(16)
C(29)-N-Ni	134.64(15)
C(28)-N-Ni	129.95(15)
C(1)-B-C(8)	109.86(18)
C(1)-B-C(9)	106.71(18)
C(8)-B-C(9)	111.62(19)
C(1)-B-C(7)	110.78(19)
C(8)-B-C(7)	112.14(18)
C(9)-B-C(7)	105.53(18)
C(2)-C(1)-C(6)	114.2(2)
C(2)-C(1)-B	121.4(2)
C(6)-C(1)-B	124.0(2)
C(3)-C(2)-C(1)	123.6(2)
C(3)-C(2)-H(2)	118.2
C(1)-C(2)-H(2)	118.2
C(4)-C(3)-C(2)	119.8(2)
C(4)-C(3)-H(3)	120.1
C(2)-C(3)-H(3)	120.1
C(5)-C(4)-C(3)	119.4(2)
C(5)-C(4)-H(4)	120.3
C(3)-C(4)-H(4)	120.3
C(4)-C(5)-C(6)	120.3(2)
C(4)-C(5)-H(5)	119.9
C(6)-C(5)-H(5)	119.9
C(5)-C(6)-C(1)	122.8(2)
C(5)-C(6)-H(6)	118.6
C(1)-C(6)-H(6)	118.6
B-C(7)-P(1)	117.13(15)
B-C(7)-H(7A)	108.0
P(1)-C(7)-H(7A)	108.0
B-C(7)-H(7B)	108.0
P(1)-C(7)-H(7B)	108.0
H(7A)-C(7)-H(7B)	107.3
B-C(8)-P(2)	120.71(15)
B-C(8)-H(8A)	107.1
P(2)-C(8)-H(8A)	107.1
B-C(8)-H(8B)	107.1
P(2)-C(8)-H(8B)	107.1
H(8A)-C(8)-H(8B)	106.8
B-C(9)-P(3)	118.77(15)
B-C(9)-H(9A)	107.6
P(3)-C(9)-H(9A)	107.6
B-C(9)-H(9B)	107.6
P(3)-C(9)-H(9B)	107.6
H(9A)-C(9)-H(9B)	107.1
C(12)-C(10)-C(11)	111.6(2)
C(12)-C(10)-P(1)	113.51(19)
C(11)-C(10)-P(1)	112.58(18)
C(12)-C(10)-H(10)	106.2
C(11)-C(10)-H(10)	106.2
P(1)-C(10)-H(10)	106.2
C(10)-C(11)-H(11A)	109.5
C(10)-C(11)-H(11B)	109.5
H(11A)-C(11)-H(11B)	109.5
C(10)-C(11)-H(11C)	109.5
H(11A)-C(11)-H(11C)	109.5
H(11B)-C(11)-H(11C)	109.5
C(10)-C(12)-H(12A)	109.5
C(10)-C(12)-H(12B)	109.5
H(12A)-C(12)-H(12B)	109.5
C(10)-C(12)-H(12C)	109.5
H(12A)-C(12)-H(12C)	109.5
H(12B)-C(12)-H(12C)	109.5
C(14)-C(13)-C(15)	111.2(2)
C(14)-C(13)-P(1)	109.87(19)
C(15)-C(13)-P(1)	112.20(19)
C(14)-C(13)-H(13)	107.8
C(15)-C(13)-H(13)	107.8
P(1)-C(13)-H(13)	107.8
C(13)-C(14)-H(14A)	109.5
C(13)-C(14)-H(14B)	109.5
H(14A)-C(14)-H(14B)	109.5
C(13)-C(14)-H(14C)	109.5
H(14A)-C(14)-H(14C)	109.5
H(14B)-C(14)-H(14C)	109.5
C(13)-C(15)-H(15A)	109.5
C(13)-C(15)-H(15B)	109.5
H(15A)-C(15)-H(15B)	109.5
C(13)-C(15)-H(15C)	109.5
H(15A)-C(15)-H(15C)	109.5
H(15B)-C(15)-H(15C)	109.5
C(18)-C(16)-C(17)	110.1(2)
C(18)-C(16)-P(2)	113.82(16)
C(17)-C(16)-P(2)	109.74(17)
C(18)-C(16)-H(16)	107.7
C(17)-C(16)-H(16)	107.7
P(2)-C(16)-H(16)	107.7
C(16)-C(17)-H(17A)	109.5
C(16)-C(17)-H(17B)	109.5
H(17A)-C(17)-H(17B)	109.5
C(16)-C(17)-H(17C)	109.5
H(17A)-C(17)-H(17C)	109.5
H(17B)-C(17)-H(17C)	109.5
C(16)-C(18)-H(18A)	109.5

C(16)-C(18)-H(18B)	109.5	C(25)-C(27)-H(27B)	109.5
H(18A)-C(18)-H(18B)	109.5	H(27A)-C(27)-H(27B)	109.5
C(16)-C(18)-H(18C)	109.5	C(25)-C(27)-H(27C)	109.5
H(18A)-C(18)-H(18C)	109.5	H(27A)-C(27)-H(27C)	109.5
H(18B)-C(18)-H(18C)	109.5	H(27B)-C(27)-H(27C)	109.5
C(20)-C(19)-H(19A)	109.5	N-C(28)-C(30)	98.80(17)
C(20)-C(19)-H(19B)	109.5	N-C(28)-C(36)	98.52(18)
H(19A)-C(19)-H(19B)	109.5	C(30)-C(28)-C(36)	108.70(19)
C(20)-C(19)-H(19C)	109.5	N-C(28)-H(28)	116.1
H(19A)-C(19)-H(19C)	109.5	C(30)-C(28)-H(28)	116.1
H(19B)-C(19)-H(19C)	109.5	C(36)-C(28)-H(28)	116.1
C(21)-C(20)-C(19)	112.8(2)	N-C(29)-C(35)	98.99(18)
C(21)-C(20)-P(2)	113.10(17)	N-C(29)-C(41)	98.84(18)
C(19)-C(20)-P(2)	113.06(17)	C(35)-C(29)-C(41)	107.70(19)
C(21)-C(20)-H(20)	105.7	N-C(29)-H(29)	116.2
C(19)-C(20)-H(20)	105.7	C(35)-C(29)-H(29)	116.2
P(2)-C(20)-H(20)	105.7	C(41)-C(29)-H(29)	116.2
C(20)-C(21)-H(21A)	109.5	C(31)-C(30)-C(35)	120.7(2)
C(20)-C(21)-H(21B)	109.5	C(31)-C(30)-C(28)	133.7(2)
H(21A)-C(21)-H(21B)	109.5	C(35)-C(30)-C(28)	105.5(2)
C(20)-C(21)-H(21C)	109.5	C(30)-C(31)-C(32)	117.5(3)
H(21A)-C(21)-H(21C)	109.5	C(30)-C(31)-H(31)	121.2
H(21B)-C(21)-H(21C)	109.5	C(32)-C(31)-H(31)	121.2
C(23)-C(22)-C(24)	111.2(2)	C(33)-C(32)-C(31)	122.0(3)
C(23)-C(22)-P(3)	108.40(19)	C(33)-C(32)-H(32)	119.0
C(24)-C(22)-P(3)	118.26(18)	C(31)-C(32)-H(32)	119.0
C(23)-C(22)-H(22)	106.0	C(32)-C(33)-C(34)	120.7(3)
C(24)-C(22)-H(22)	106.0	C(32)-C(33)-H(33)	119.7
P(3)-C(22)-H(22)	106.0	C(34)-C(33)-H(33)	119.7
C(22)-C(23)-H(23A)	109.5	C(35)-C(34)-C(33)	118.2(3)
C(22)-C(23)-H(23B)	109.5	C(35)-C(34)-H(34)	120.9
H(23A)-C(23)-H(23B)	109.5	C(33)-C(34)-H(34)	120.9
C(22)-C(23)-H(23C)	109.5	C(34)-C(35)-C(30)	120.8(2)
H(23A)-C(23)-H(23C)	109.5	C(34)-C(35)-C(29)	133.3(2)
H(23B)-C(23)-H(23C)	109.5	C(30)-C(35)-C(29)	105.8(2)
C(22)-C(24)-H(24A)	109.5	C(37)-C(36)-C(41)	121.8(2)
C(22)-C(24)-H(24B)	109.5	C(37)-C(36)-C(28)	133.0(2)
H(24A)-C(24)-H(24B)	109.5	C(41)-C(36)-C(28)	105.1(2)
C(22)-C(24)-H(24C)	109.5	C(36)-C(37)-C(38)	117.4(3)
H(24A)-C(24)-H(24C)	109.5	C(36)-C(37)-H(37)	121.3
H(24B)-C(24)-H(24C)	109.5	C(38)-C(37)-H(37)	121.3
C(27)-C(25)-C(26)	108.4(2)	C(39)-C(38)-C(37)	121.3(3)
C(27)-C(25)-P(3)	117.40(19)	C(39)-C(38)-H(38)	119.4
C(26)-C(25)-P(3)	107.50(19)	C(37)-C(38)-H(38)	119.4
C(27)-C(25)-H(25)	107.7	C(38)-C(39)-C(40)	121.6(3)
C(26)-C(25)-H(25)	107.7	C(38)-C(39)-H(39)	119.2
P(3)-C(25)-H(25)	107.7	C(40)-C(39)-H(39)	119.2
C(25)-C(26)-H(26A)	109.5	C(41)-C(40)-C(39)	117.6(3)
C(25)-C(26)-H(26B)	109.5	C(41)-C(40)-H(40)	121.2
H(26A)-C(26)-H(26B)	109.5	C(39)-C(40)-H(40)	121.2
C(25)-C(26)-H(26C)	109.5	C(40)-C(41)-C(36)	120.3(3)
H(26A)-C(26)-H(26C)	109.5	C(40)-C(41)-C(29)	133.8(3)
H(26B)-C(26)-H(26C)	109.5	C(36)-C(41)-C(29)	105.8(2)
C(25)-C(27)-H(27A)	109.5		

Table 47. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for 11. The anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2 a^{*2} U^{11} + ... + 2\ h\ k\ a^*\ b^*\ U^{12}]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Ni	25(1)	22(1)	17(1)	-2(1)	-2(1)	2(1)
P(1)	25(1)	28(1)	22(1)	-3(1)	2(1)	4(1)
P(2)	25(1)	21(1)	15(1)	-1(1)	1(1)	3(1)
P(3)	28(1)	28(1)	35(1)	-3(1)	6(1)	-1(1)
N	25(1)	25(1)	21(1)	-1(1)	-2(1)	1(1)
B	25(2)	20(1)	18(1)	-4(1)	1(1)	2(1)
C(1)	21(1)	23(1)	22(1)	-2(1)	2(1)	-3(1)
C(2)	39(2)	28(1)	25(1)	-1(1)	4(1)	0(1)
C(3)	39(2)	39(2)	26(1)	-9(1)	7(1)	-3(1)
C(4)	32(2)	46(2)	19(1)	4(1)	4(1)	-4(1)
C(5)	40(2)	31(2)	27(1)	6(1)	2(1)	4(1)
C(6)	34(2)	30(1)	20(1)	-2(1)	7(1)	4(1)
C(7)	29(1)	24(1)	20(1)	-5(1)	3(1)	3(1)
C(8)	22(1)	22(1)	15(1)	1(1)	-1(1)	1(1)
C(9)	29(2)	24(1)	20(1)	1(1)	1(1)	3(1)
C(10)	35(2)	40(2)	28(1)	-1(1)	6(1)	-7(1)
C(11)	48(2)	50(2)	42(2)	2(1)	7(1)	-16(2)
C(12)	65(2)	69(2)	39(2)	-5(2)	26(2)	-13(2)
C(13)	29(2)	51(2)	39(2)	-13(1)	1(1)	13(1)
C(14)	54(2)	56(2)	52(2)	15(2)	4(2)	28(2)
C(15)	29(2)	78(2)	82(3)	-28(2)	-10(2)	17(2)
C(16)	26(1)	27(1)	26(1)	-6(1)	0(1)	8(1)
C(17)	47(2)	23(1)	29(1)	-4(1)	-2(1)	6(1)
C(18)	34(2)	39(2)	26(1)	-10(1)	5(1)	6(1)
C(19)	54(2)	37(2)	24(1)	7(1)	7(1)	1(1)
C(20)	38(2)	26(1)	20(1)	4(1)	6(1)	-3(1)
C(21)	40(2)	45(2)	32(2)	1(1)	9(1)	-8(1)
C(22)	28(2)	33(2)	39(2)	0(1)	-3(1)	0(1)
C(23)	40(2)	49(2)	58(2)	-5(2)	-9(2)	11(2)
C(24)	43(2)	45(2)	31(2)	0(1)	-3(1)	5(1)
C(25)	28(2)	33(2)	44(2)	-1(1)	6(1)	-8(1)
C(26)	108(3)	44(2)	80(3)	-8(2)	57(2)	-19(2)
C(27)	54(2)	38(2)	39(2)	2(1)	6(1)	-12(1)
C(28)	31(2)	24(1)	20(1)	1(1)	3(1)	-3(1)
C(29)	31(2)	29(1)	24(1)	6(1)	-4(1)	-6(1)
C(30)	26(1)	31(1)	22(1)	-7(1)	2(1)	-1(1)
C(31)	33(2)	39(2)	38(2)	-5(1)	13(1)	-2(1)
C(32)	25(2)	54(2)	68(2)	-13(2)	12(2)	-3(1)
C(33)	33(2)	50(2)	69(2)	1(2)	-8(2)	5(2)
C(34)	38(2)	40(2)	45(2)	4(1)	-11(1)	-2(1)
C(35)	29(2)	31(1)	24(1)	-2(1)	-4(1)	-2(1)
C(36)	23(1)	32(1)	25(1)	-9(1)	2(1)	-9(1)
C(37)	24(2)	39(2)	47(2)	-17(1)	5(1)	-7(1)
C(38)	30(2)	59(2)	60(2)	-29(2)	10(2)	-10(2)
C(39)	40(2)	85(3)	41(2)	-33(2)	19(2)	-23(2)
C(40)	41(2)	64(2)	27(2)	-4(1)	3(1)	-25(2)
C(41)	24(2)	44(2)	21(1)	-6(1)	-1(1)	-12(1)

Table 48. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for 11.

	x	y	z	U(eq)
H(2)	5343	438	26	36
H(3)	5109	638	-1742	41
H(4)	4398	1429	-2322	39
H(5)	3944	2014	-1116	39
H(6)	4138	1806	651	33
H(7A)	6286	453	1655	29
H(7B)	5851	347	2738	29
H(8A)	3697	1429	2455	24
H(8B)	4802	1703	2205	24
H(9A)	3963	261	2422	29
H(9B)	3882	220	1183	29
H(10)	6647	1616	1613	41
H(11A)	8775	1849	2838	70
H(11B)	7602	2107	2974	70
H(11C)	8132	2204	1930	70
H(12A)	7986	1530	537	84
H(12B)	7551	975	777	84
H(12C)	8743	1172	1367	84
H(13)	8558	457	2567	48
H(14A)	8803	-57	4072	82
H(14B)	7500	-32	3570	82
H(14C)	7960	295	4592	82
H(15A)	9220	1114	4315	97
H(15B)	9688	1118	3223	97
H(15C)	10021	665	4038	97
H(16)	3715	2030	4106	32
H(17A)	4753	2780	4122	51
H(17B)	5018	2435	3172	51
H(17C)	5908	2469	4231	51
H(18A)	5476	1995	5875	50
H(18B)	4220	1789	5847	50
H(18C)	4448	2386	5778	50
H(19A)	5123	998	6072	57
H(19B)	5878	630	5484	57
H(19C)	4749	421	5842	57
H(20)	4468	579	4035	33
H(21A)	2862	643	4789	58
H(21B)	2792	1048	3859	58
H(21C)	3100	1230	5051	58
H(22)	2400	1083	26	41
H(23A)	525	1159	-691	76
H(23B)	660	1287	534	76
H(23C)	168	749	108	76
H(24A)	1442	122	-595	61
H(24B)	2764	232	-474	61
H(24C)	1906	532	-1333	61
H(25)	787	60	1369	42
H(26A)	1015	-315	3026	109
H(26B)	1131	287	3160	109
H(26C)	2233	-62	3331	109
H(27A)	2802	-512	1870	66
H(27B)	2206	-409	691	66
H(27C)	1570	-732	1466	66

H(28)	8130	2394	4987	30
H(29)	7879	1111	6695	34
H(31)	10545	2493	5509	43
H(32)	12152	2038	6263	58
H(33)	12012	1319	7224	63
H(34)	10247	1003	7449	52
H(37)	7274	3080	6390	44
H(38)	6400	3099	7896	59
H(39)	6325	2389	8898	65
H(40)	7066	1608	8428	53

Figure 9. Fully-labeled displacement ellipsoid (50%) representation of $[PhB(CH_2PPh_2)_3]Ni(PPh_3) \cdot C_{9.95}$ (**12· $C_{9.95}$**) (hydrogens omitted for clarity).

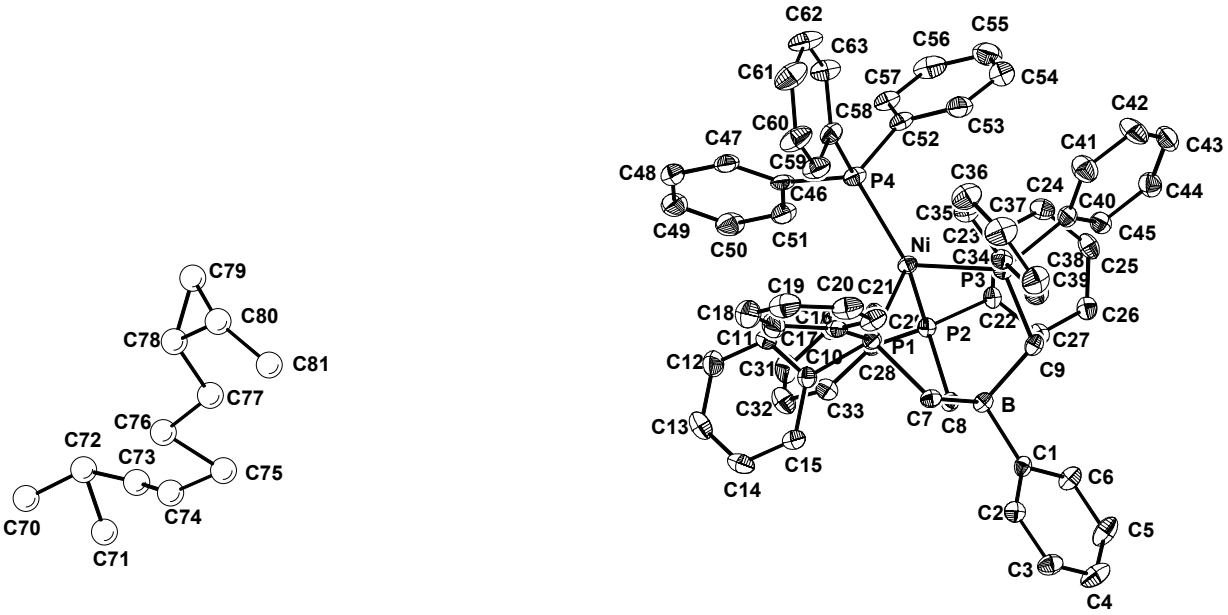


Table 49. Crystal data and structure refinement for 12· $C_{9.95}$.

Empirical formula	$C_{72.95}H_{56}BNiP_4$	
Moiety formula	$C_{63}H_{56}BNiP_4 \cdot C_{9.95}$	
Formula weight	1125.93	
Crystal habit	rough plate	
Crystal color	yellow	
Crystal size	0.22 x 0.19 x 0.19 mm^3	
Data Collection		
Type of diffractometer	Bruker P4	
Wavelength	0.71073 Å	
Temperature	98(2) K	
Unit cell dimensions	a = 19.9842(13) Å	α = 90°
	b = 17.8132(11) Å	β = 90°
	c = 33.699(2) Å	γ = 90°
Volume	11996.4(13) $Å^3$	
Z	8	
Crystal system	Orthorhombic	
Space group	Pbca	
Density (calculated)	1.247 g/cm^3	
F(000)	4693	
θ range for data collection	1.58 to 28.55°	
Completeness to θ = 28.55°	95.0%	
Index ranges	$-25 \le h \le 26$, $-23 \le k \le 23$, $-45 \le l \le 42$	
Reflections collected	126093	
Independent reflections	14493 [R(int) = 0.0873]	
Absorption coefficient	0.473 mm^{-1}	
Absorption correction	None	
Structure solution and refinement		
Structure solution program	SHELXS-97 (Sheldrick, 1990)	
Primary solution method	direct methods	
Secondary solution method	difference Fourier map	
Hydrogen placement	calculated positions	
Structure refinement program	SHELXL-97 (Sheldrick, 1997)	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	14493 / 13 / 682	
Goodness-of-fit on F^2	2.299	
Final R indices [$I>2\sigma(I)$]	R1 = 0.0573, wR2 = 0.0951	
R indices (all data)	R1 = 0.0977, wR2 = 0.0981	
Type of weighting scheme used	calculated	
Weighting scheme used	calc $w=1/[\sigma^2(F_o^2)]$	
Max shift/error	0.268	
Average shift/error	0.001	
Largest diff. peak and hole	1.427 and -0.548 $e \cdot Å^{-3}$	

Additional refinement details: The structure contains a highly disordered solvent site occupied by a pentane chain. As a consequence of the disorder, several isotropic carbon positions have been refined with positional restraints and partial occupations. The remainder of the structure has been refined anisotropically.

Table 50. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$ x 10^3) for 12·$C_{9.95}$. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
Ni	9999(5)	5974(5)	6535(3)	16(2)
P(1)	9242(10)	6820(11)	6772(6)	18(5)
P(2)	9774(9)	5071(11)	6996(6)	16(4)
P(3)	10853(9)	6529(11)	6869(6)	18(5)
P(4)	10041(10)	5719(10)	5882(6)	21(5)
B	9870(40)	6400(40)	7530(30)	20(20)
C(1)	9850(30)	6560(40)	8010(20)	17(17)
C(2)	9520(30)	7150(40)	8190(20)	20(18)
C(3)	9530(40)	7260(40)	8600(20)	25(19)
C(4)	9870(40)	6770(50)	8840(20)	30(20)
C(5)	10200(40)	6170(50)	8670(20)	30(20)
C(6)	10200(40)	6070(40)	8270(20)	25(19)
C(7)	9440(40)	7050(40)	7290(20)	18(17)
C(8)	9550(30)	5550(40)	7460(20)	17(17)
C(9)	10680(30)	6440(40)	7390(20)	18(17)
C(10)	8420(30)	6370(40)	6770(20)	20(18)
C(11)	8260(40)	5920(40)	6440(20)	25(19)
C(12)	7630(40)	5600(50)	6400(30)	30(20)
C(13)	7150(40)	5730(50)	6690(30)	30(20)
C(14)	7300(40)	6170(40)	7010(30)	30(20)
C(15)	7930(40)	6490(40)	7050(20)	22(18)
C(16)	9010(40)	7720(40)	6530(20)	20(17)
C(17)	8460(40)	7790(50)	6290(20)	30(20)
C(18)	8310(40)	8460(50)	6100(30)	40(20)
C(19)	8710(40)	9080(50)	6150(20)	40(20)
C(20)	9270(40)	9020(50)	6390(20)	30(20)
C(21)	9420(40)	8350(40)	6580(20)	30(20)
C(22)	10530(30)	4520(40)	7100(20)	16(17)
C(23)	10930(30)	4300(40)	6770(20)	20(17)
C(24)	11500(40)	3870(40)	6830(20)	24(19)
C(25)	11700(40)	3670(40)	7210(20)	24(19)
C(26)	11310(40)	3880(40)	7530(20)	22(19)
C(27)	10730(40)	4300(40)	7470(20)	19(17)
C(28)	9160(30)	4310(40)	6950(20)	17(16)
C(29)	9340(40)	3580(40)	6820(20)	21(18)
C(30)	8860(40)	3030(40)	6770(20)	25(19)
C(31)	8200(40)	3180(40)	6830(20)	30(20)
C(32)	8000(40)	3890(40)	6950(20)	30(20)
C(33)	8480(30)	4450(40)	7010(20)	21(18)
C(34)	10930(30)	7530(40)	6750(20)	19(17)
C(35)	10900(40)	7730(40)	6350(20)	25(19)
C(36)	11010(40)	8470(50)	6230(30)	30(20)
C(37)	11130(40)	9010(50)	6510(30)	40(20)
C(38)	11140(40)	8830(40)	6910(30)	30(20)
C(39)	11050(40)	8090(40)	7030(20)	26(19)
C(40)	11750(40)	6270(40)	6820(20)	21(18)
C(41)	12200(40)	6700(50)	6600(30)	30(20)
C(42)	12870(40)	6510(50)	6580(30)	40(20)
C(43)	13110(40)	5890(50)	6780(30)	30(20)
C(44)	12670(40)	5450(50)	6990(20)	30(20)
C(45)	12000(40)	5640(40)	7010(20)	22(18)
C(46)	9330(40)	5180(40)	5690(20)	22(18)
C(47)	8940(40)	5410(50)	5370(20)	30(20)

C(48)	8380(40)	5010(50)	5260(20)	30(20)
C(49)	8200(40)	4370(50)	5470(30)	40(20)
C(50)	8580(40)	4130(50)	5790(20)	30(20)
C(51)	9140(40)	4530(40)	5900(20)	27(19)
C(52)	10780(40)	5140(40)	5780(20)	23(18)
C(53)	11400(40)	5440(50)	5890(20)	30(20)
C(54)	11970(40)	5000(50)	5890(20)	40(20)
C(55)	11940(40)	4260(50)	5770(30)	40(20)
C(56)	11330(50)	3960(50)	5660(20)	40(20)
C(57)	10750(40)	4390(40)	5660(20)	26(19)
C(58)	10100(40)	6490(40)	5520(20)	23(18)
C(59)	9780(40)	7150(50)	5620(20)	30(20)
C(60)	9780(40)	7750(50)	5360(30)	40(20)
C(61)	10110(50)	7690(50)	5000(30)	40(20)
C(62)	10430(40)	7030(50)	4900(30)	40(20)
C(63)	10430(40)	6430(50)	5160(20)	30(20)
C(78)	2800(110)	3200(120)	4510(70)	160(140)
C(75)	2450(150)	2140(160)	5440(80)	200(200)
C(77)	2800(150)	2860(150)	4950(80)	200(200)
C(76)	2140(140)	2360(150)	5010(80)	170(180)
C(80)	3330(130)	3830(150)	4520(90)	170(190)
C(71)	950(180)	100(190)	5470(160)	300(300)
C(72)	1100(300)	300(200)	5050(170)	400(500)
C(81)	3600(200)	4300(300)	4910(120)	300(400)
C(79)	3350(170)	3200(200)	4230(100)	200(200)
C(74)	1820(180)	1700(200)	5400(110)	300(300)
C(73)	1600(200)	900(200)	5270(150)	200(300)
C(70)	400(300)	0(300)	5000(200)	400(500)

Table 51. Selected bond lengths [Å] and angles [°] for 12· $C_{9.95}$.

Ni-P(4)	2.25(2)	P(4)-Ni-P(3)	123.0(8)
Ni-P(3)	2.27(2)	P(4)-Ni-P(1)	120.1(8)
Ni-P(1)	2.28(2)	P(3)-Ni-P(1)	92.2(8)
Ni-P(2)	2.28(2)	P(4)-Ni-P(2)	122.1(8)
Ni-B	3.44(9)	P(3)-Ni-P(2)	96.8(8)
		P(1)-Ni-P(2)	95.6(8)

Table 52. Bond lengths [Å] and angles [°] for 12· $C_{9.95}$.

Ni-P(4)	2.25(2)	C(19)-H(19)	0.9500
Ni-P(3)	2.27(2)	C(20)-C(21)	1.39(10)
Ni-P(1)	2.28(2)	C(20)-H(20)	0.9500
Ni-P(2)	2.28(2)	C(21)-H(21)	0.9500
Ni-B	3.44(9)	C(22)-C(27)	1.39(9)
P(1)-C(7)	1.82(7)	C(22)-C(23)	1.40(10)
P(1)-C(10)	1.83(7)	C(23)-C(24)	1.39(9)
P(1)-C(16)	1.85(7)	C(23)-H(23)	0.9500
P(2)-C(8)	1.82(7)	C(24)-C(25)	1.38(10)
P(2)-C(22)	1.84(7)	C(24)-H(24)	0.9500
P(2)-C(28)	1.84(7)	C(25)-C(26)	1.38(10)
P(3)-C(9)	1.81(7)	C(25)-H(25)	0.9500
P(3)-C(34)	1.84(7)	C(26)-C(27)	1.39(9)
P(3)-C(40)	1.85(8)	C(26)-H(26)	0.9500
P(4)-C(58)	1.83(8)	C(27)-H(27)	0.9500
P(4)-C(52)	1.83(8)	C(28)-C(33)	1.40(9)
P(4)-C(46)	1.83(8)	C(28)-C(29)	1.40(9)
B-C(1)	1.64(11)	C(29)-C(30)	1.39(9)
B-C(7)	1.66(10)	C(29)-H(29)	0.9500
B-C(8)	1.67(10)	C(30)-C(31)	1.38(10)
B-C(9)	1.67(10)	C(30)-H(30)	0.9500
C(1)-C(2)	1.40(9)	C(31)-C(32)	1.38(10)
C(1)-C(6)	1.41(10)	C(31)-H(31)	0.9500
C(2)-C(3)	1.39(10)	C(32)-C(33)	1.39(10)
C(2)-H(2)	0.9500	C(32)-H(32)	0.9500
C(3)-C(4)	1.38(10)	C(33)-H(33)	0.9500
C(3)-H(3)	0.9500	C(34)-C(35)	1.39(10)
C(4)-C(5)	1.38(11)	C(34)-C(39)	1.39(10)
C(4)-H(4)	0.9500	C(35)-C(36)	1.38(10)
C(5)-C(6)	1.38(10)	C(35)-H(35)	0.9500
C(5)-H(5)	0.9500	C(36)-C(37)	1.38(11)
C(6)-H(6)	0.9500	C(36)-H(36)	0.9500
C(7)-H(7A)	0.9900	C(37)-C(38)	1.38(11)
C(7)-H(7B)	0.9900	C(37)-H(37)	0.9500
C(8)-H(8A)	0.9900	C(38)-C(39)	1.38(10)
C(8)-H(8B)	0.9900	C(38)-H(38)	0.9500
C(9)-H(9A)	0.9900	C(39)-H(39)	0.9500
C(9)-H(9B)	0.9900	C(40)-C(45)	1.39(10)
C(10)-C(11)	1.39(10)	C(40)-C(41)	1.39(10)
C(10)-C(15)	1.39(10)	C(41)-C(42)	1.38(10)
C(11)-C(12)	1.39(10)	C(41)-H(41)	0.9500
C(11)-H(11)	0.9500	C(42)-C(43)	1.38(11)
C(12)-C(13)	1.37(11)	C(42)-H(42)	0.9500
C(12)-H(12)	0.9500	C(43)-C(44)	1.37(11)
C(13)-C(14)	1.38(11)	C(43)-H(43)	0.9500
C(13)-H(13)	0.9500	C(44)-C(45)	1.39(10)
C(14)-C(15)	1.39(10)	C(44)-H(44)	0.9500
C(14)-H(14)	0.9500	C(45)-H(45)	0.9500
C(15)-H(15)	0.9500	C(46)-C(47)	1.38(10)
C(16)-C(17)	1.39(10)	C(46)-C(51)	1.40(10)
C(16)-C(21)	1.40(10)	C(47)-C(48)	1.38(10)
C(17)-C(18)	1.39(11)	C(47)-H(47)	0.9500
C(17)-H(17)	0.9500	C(48)-C(49)	1.39(11)
C(18)-C(19)	1.37(12)	C(48)-H(48)	0.9500
C(18)-H(18)	0.9500	C(49)-C(50)	1.38(11)
C(19)-C(20)	1.38(11)	C(49)-H(49)	0.9500

C(50)-C(51)	1.38(10)	C(10)-P(1)-Ni	108(2)
C(50)-H(50)	0.9500	C(16)-P(1)-Ni	126(2)
C(51)-H(51)	0.9500	C(8)-P(2)-C(22)	107(3)
C(52)-C(57)	1.39(10)	C(8)-P(2)-C(28)	105(3)
C(52)-C(53)	1.40(10)	C(22)-P(2)-C(28)	100(3)
C(53)-C(54)	1.38(11)	C(8)-P(2)-Ni	107(2)
C(53)-H(53)	0.9500	C(22)-P(2)-Ni	110(2)
C(54)-C(55)	1.38(12)	C(28)-P(2)-Ni	126(2)
C(54)-H(54)	0.9500	C(9)-P(3)-C(34)	108(3)
C(55)-C(56)	1.38(12)	C(9)-P(3)-C(40)	104(3)
C(55)-H(55)	0.9500	C(34)-P(3)-C(40)	98(3)
C(56)-C(57)	1.39(11)	C(9)-P(3)-Ni	108(2)
C(56)-H(56)	0.9500	C(34)-P(3)-Ni	112(2)
C(57)-H(57)	0.9500	C(40)-P(3)-Ni	125(2)
C(58)-C(63)	1.38(10)	C(58)-P(4)-C(52)	104(3)
C(58)-C(59)	1.39(10)	C(58)-P(4)-C(46)	102(4)
C(59)-C(60)	1.38(11)	C(52)-P(4)-C(46)	105(3)
C(59)-H(59)	0.9500	C(58)-P(4)-Ni	120(3)
C(60)-C(61)	1.37(11)	C(52)-P(4)-Ni	109(2)
C(60)-H(60)	0.9500	C(46)-P(4)-Ni	115(2)
C(61)-C(62)	1.38(11)	C(1)-B-C(7)	111(6)
C(61)-H(61)	0.9500	C(1)-B-C(8)	107(6)
C(62)-C(63)	1.39(11)	C(7)-B-C(8)	111(6)
C(62)-H(62)	0.9500	C(1)-B-C(9)	106(6)
C(63)-H(63)	0.9500	C(7)-B-C(9)	110(6)
C(78)-C(79)	1.4(2)	C(8)-B-C(9)	112(6)
C(78)-C(80)	1.5(2)	C(1)-B-Ni	176(5)
C(78)-C(77)	1.6(2)	C(7)-B-Ni	73(4)
C(75)-C(74)	1.5(2)	C(8)-B-Ni	72(4)
C(75)-C(76)	1.6(2)	C(9)-B-Ni	71(4)
C(77)-C(76)	1.6(2)	C(2)-C(1)-C(6)	115(7)
C(76)-C(74)	1.9(4)	C(2)-C(1)-B	125(6)
C(80)-C(79)	1.5(2)	C(6)-C(1)-B	120(6)
C(80)-C(81)	1.6(2)	C(3)-C(2)-C(1)	123(7)
C(71)-C(72)	1.5(2)	C(3)-C(2)-H(2)	118.6
C(71)-C(70)	1.9(7)	C(1)-C(2)-H(2)	118.6
C(71)-C(73)	2.0(6)	C(4)-C(3)-C(2)	121(8)
C(72)-C(70)	1.5(2)	C(4)-C(3)-H(3)	119.7
C(72)-C(73)	1.6(3)	C(2)-C(3)-H(3)	119.7
C(72)-C(81)#1	2.0(6)	C(3)-C(4)-C(5)	119(8)
C(81)-C(72)#2	2.0(6)	C(3)-C(4)-H(4)	120.7
C(74)-C(73)	1.5(2)	C(5)-C(4)-H(4)	120.7
C(70)-C(70)#3	1.7(11)	C(4)-C(5)-C(6)	120(8)
		C(4)-C(5)-H(5)	119.8
P(4)-Ni-P(3)	123.0(8)	C(6)-C(5)-H(5)	119.8
P(4)-Ni-P(1)	120.1(8)	C(5)-C(6)-C(1)	123(7)
P(3)-Ni-P(1)	92.2(8)	C(5)-C(6)-H(6)	118.7
P(4)-Ni-P(2)	122.1(8)	C(1)-C(6)-H(6)	118.7
P(3)-Ni-P(2)	96.8(8)	B-C(7)-P(1)	115(5)
P(1)-Ni-P(2)	95.6(8)	B-C(7)-H(7A)	108.4
P(4)-Ni-B	177.6(15)	P(1)-C(7)-H(7A)	108.4
P(3)-Ni-B	58.5(14)	B-C(7)-H(7B)	108.4
P(1)-Ni-B	57.6(14)	P(1)-C(7)-H(7B)	108.4
P(2)-Ni-B	58.7(14)	H(7A)-C(7)-H(7B)	107.5
C(7)-P(1)-C(10)	107(3)	B-C(8)-P(2)	117(5)
C(7)-P(1)-C(16)	106(3)	B-C(8)-H(8A)	108.0
C(10)-P(1)-C(16)	99(3)	P(2)-C(8)-H(8A)	108.0
C(7)-P(1)-Ni	110(2)	B-C(8)-H(8B)	108.0

P(2)-C(8)-H(8B)	108.0	C(27)-C(26)-H(26)	119.7
H(8A)-C(8)-H(8B)	107.2	C(26)-C(27)-C(22)	121(7)
B-C(9)-P(3)	117(5)	C(26)-C(27)-H(27)	119.6
B-C(9)-H(9A)	108.1	C(22)-C(27)-H(27)	119.6
P(3)-C(9)-H(9A)	108.1	C(33)-C(28)-C(29)	118(6)
B-C(9)-H(9B)	108.1	C(33)-C(28)-P(2)	120(5)
P(3)-C(9)-H(9B)	108.1	C(29)-C(28)-P(2)	122(5)
H(9A)-C(9)-H(9B)	107.3	C(30)-C(29)-C(28)	121(7)
C(11)-C(10)-C(15)	118(7)	C(30)-C(29)-H(29)	119.4
C(11)-C(10)-P(1)	118(6)	C(28)-C(29)-H(29)	119.4
C(15)-C(10)-P(1)	124(6)	C(31)-C(30)-C(29)	120(7)
C(12)-C(11)-C(10)	122(7)	C(31)-C(30)-H(30)	120.0
C(12)-C(11)-H(11)	119.2	C(29)-C(30)-H(30)	120.0
C(10)-C(11)-H(11)	119.2	C(30)-C(31)-C(32)	120(7)
C(13)-C(12)-C(11)	120(8)	C(30)-C(31)-H(31)	120.0
C(13)-C(12)-H(12)	120.0	C(32)-C(31)-H(31)	120.0
C(11)-C(12)-H(12)	120.0	C(31)-C(32)-C(33)	120(7)
C(12)-C(13)-C(14)	119(8)	C(31)-C(32)-H(32)	119.8
C(12)-C(13)-H(13)	120.3	C(33)-C(32)-H(32)	119.8
C(14)-C(13)-H(13)	120.3	C(32)-C(33)-C(28)	121(7)
C(13)-C(14)-C(15)	121(7)	C(32)-C(33)-H(33)	119.7
C(13)-C(14)-H(14)	119.7	C(28)-C(33)-H(33)	119.7
C(15)-C(14)-H(14)	119.7	C(35)-C(34)-C(39)	118(7)
C(10)-C(15)-C(14)	120(7)	C(35)-C(34)-P(3)	117(6)
C(10)-C(15)-H(15)	119.8	C(39)-C(34)-P(3)	124(6)
C(14)-C(15)-H(15)	119.8	C(36)-C(35)-C(34)	122(8)
C(17)-C(16)-C(21)	117(7)	C(36)-C(35)-H(35)	119.2
C(17)-C(16)-P(1)	122(6)	C(34)-C(35)-H(35)	119.2
C(21)-C(16)-P(1)	120(6)	C(37)-C(36)-C(35)	119(8)
C(18)-C(17)-C(16)	121(8)	C(37)-C(36)-H(36)	120.3
C(18)-C(17)-H(17)	119.3	C(35)-C(36)-H(36)	120.3
C(16)-C(17)-H(17)	119.3	C(36)-C(37)-C(38)	120(8)
C(19)-C(18)-C(17)	121(8)	C(36)-C(37)-H(37)	120.0
C(19)-C(18)-H(18)	119.6	C(38)-C(37)-H(37)	120.0
C(17)-C(18)-H(18)	119.6	C(37)-C(38)-C(39)	120(8)
C(18)-C(19)-C(20)	119(8)	C(37)-C(38)-H(38)	119.8
C(18)-C(19)-H(19)	120.5	C(39)-C(38)-H(38)	119.8
C(20)-C(19)-H(19)	120.5	C(38)-C(39)-C(34)	120(8)
C(19)-C(20)-C(21)	120(8)	C(38)-C(39)-H(39)	119.9
C(19)-C(20)-H(20)	119.8	C(34)-C(39)-H(39)	119.9
C(21)-C(20)-H(20)	119.8	C(45)-C(40)-C(41)	117(7)
C(20)-C(21)-C(16)	121(8)	C(45)-C(40)-P(3)	120(6)
C(20)-C(21)-H(21)	119.5	C(41)-C(40)-P(3)	123(6)
C(16)-C(21)-H(21)	119.5	C(42)-C(41)-C(40)	121(8)
C(27)-C(22)-C(23)	118(7)	C(42)-C(41)-H(41)	119.3
C(27)-C(22)-P(2)	124(6)	C(40)-C(41)-H(41)	119.3
C(23)-C(22)-P(2)	118(6)	C(43)-C(42)-C(41)	121(8)
C(24)-C(23)-C(22)	121(7)	C(43)-C(42)-H(42)	119.6
C(24)-C(23)-H(23)	119.5	C(41)-C(42)-H(42)	119.6
C(22)-C(23)-H(23)	119.5	C(44)-C(43)-C(42)	118(8)
C(25)-C(24)-C(23)	120(7)	C(44)-C(43)-H(43)	120.8
C(25)-C(24)-H(24)	120.0	C(42)-C(43)-H(43)	120.8
C(23)-C(24)-H(24)	120.0	C(43)-C(44)-C(45)	121(8)
C(26)-C(25)-C(24)	120(7)	C(43)-C(44)-H(44)	119.5
C(26)-C(25)-H(25)	120.2	C(45)-C(44)-H(44)	119.5
C(24)-C(25)-H(25)	120.2	C(44)-C(45)-C(40)	121(7)
C(25)-C(26)-C(27)	121(7)	C(44)-C(45)-H(45)	119.5
C(25)-C(26)-H(26)	119.7	C(40)-C(45)-H(45)	119.5

C(47)-C(46)-C(51)	118(7)	C(61)-C(60)-H(60)	119.9
C(47)-C(46)-P(4)	123(6)	C(59)-C(60)-H(60)	119.9
C(51)-C(46)-P(4)	118(6)	C(60)-C(61)-C(62)	120(8)
C(46)-C(47)-C(48)	121(8)	C(60)-C(61)-H(61)	120.0
C(46)-C(47)-H(47)	119.7	C(62)-C(61)-H(61)	120.0
C(48)-C(47)-H(47)	119.7	C(61)-C(62)-C(63)	120(8)
C(47)-C(48)-C(49)	120(8)	C(61)-C(62)-H(62)	120.1
C(47)-C(48)-H(48)	119.9	C(63)-C(62)-H(62)	120.1
C(49)-C(48)-H(48)	119.9	C(58)-C(63)-C(62)	120(8)
C(50)-C(49)-C(48)	120(8)	C(58)-C(63)-H(63)	119.8
C(50)-C(49)-H(49)	120.0	C(62)-C(63)-H(63)	119.8
C(48)-C(49)-H(49)	120.0	C(79)-C(78)-C(80)	62(10)
C(49)-C(50)-C(51)	120(8)	C(79)-C(78)-C(77)	125(10)
C(49)-C(50)-H(50)	120.1	C(80)-C(78)-C(77)	105(10)
C(51)-C(50)-H(50)	120.1	C(74)-C(75)-C(76)	75(10)
C(50)-C(51)-C(46)	121(8)	C(76)-C(77)-C(78)	109(10)
C(50)-C(51)-H(51)	119.5	C(77)-C(76)-C(75)	86(10)
C(46)-C(51)-H(51)	119.5	C(77)-C(76)-C(74)	136(10)
C(57)-C(52)-C(53)	119(7)	C(75)-C(76)-C(74)	50(10)
C(57)-C(52)-P(4)	124(6)	C(79)-C(80)-C(78)	56(10)
C(53)-C(52)-P(4)	117(6)	C(79)-C(80)-C(81)	153(10)
C(54)-C(53)-C(52)	121(8)	C(78)-C(80)-C(81)	124(10)
C(54)-C(53)-H(53)	119.5	C(72)-C(71)-C(70)	53(10)
C(52)-C(53)-H(53)	119.5	C(72)-C(71)-C(73)	51(10)
C(55)-C(54)-C(53)	120(8)	C(70)-C(71)-C(73)	99(10)
C(55)-C(54)-H(54)	120.0	C(71)-C(72)-C(70)	76(10)
C(53)-C(54)-H(54)	120.0	C(71)-C(72)-C(73)	80(10)
C(54)-C(55)-C(56)	120(8)	C(70)-C(72)-C(73)	143(10)
C(54)-C(55)-H(55)	120.1	C(71)-C(72)-C(81)#1	96(10)
C(56)-C(55)-H(55)	120.1	C(70)-C(72)-C(81)#1	85(10)
C(55)-C(56)-C(57)	121(9)	C(73)-C(72)-C(81)#1	125(10)
C(55)-C(56)-H(56)	119.7	C(80)-C(81)-C(72)#2	136(10)
C(57)-C(56)-H(56)	119.7	C(78)-C(79)-C(80)	62(10)
C(56)-C(57)-C(52)	120(8)	C(75)-C(74)-C(73)	143(10)
C(56)-C(57)-H(57)	120.0	C(75)-C(74)-C(76)	55(10)
C(52)-C(57)-H(57)	120.0	C(73)-C(74)-C(76)	119(10)
C(63)-C(58)-C(59)	119(7)	C(74)-C(73)-C(72)	160(10)
C(63)-C(58)-P(4)	124(6)	C(74)-C(73)-C(71)	138(10)
C(59)-C(58)-P(4)	117(6)	C(72)-C(73)-C(71)	49(10)
C(60)-C(59)-C(58)	121(8)	C(72)-C(70)-C(70)#3	152(10)
C(60)-C(59)-H(59)	119.7	C(72)-C(70)-C(71)	52(10)
C(58)-C(59)-H(59)	119.7	C(70)#3-C(70)-C(71)	126(10)
C(61)-C(60)-C(59)	120(8)		

Symmetry transformations used to generate equivalent atoms:
#1 -x+1/2,y-1/2,z #2 -x+1/2,y+1/2,z #3 -x,-y,-z+1

Table 53. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for 12· $C_{9.95}$. The anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2 a^{*2} U^{11} + ... + 2\ h\ k\ a^*\ b^*\ U^{12}]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Ni	19(5)	15(4)	15(5)	-1(4)	1(4)	0(4)
P(1)	18(11)	20(10)	15(11)	-1(9)	-1(9)	3(8)
P(2)	17(10)	14(10)	17(11)	-1(9)	-1(8)	0(8)
P(3)	19(11)	16(10)	18(12)	0(9)	1(9)	-1(8)
P(4)	27(11)	21(10)	16(11)	-2(9)	3(10)	-4(10)
B	20(50)	10(50)	20(50)	0(40)	0(40)	0(40)
C(1)	20(40)	20(40)	20(40)	0(30)	0(30)	0(30)
C(2)	20(40)	20(40)	20(50)	0(40)	0(30)	0(30)
C(3)	30(50)	20(40)	20(50)	-10(40)	0(40)	0(40)
C(4)	50(60)	30(50)	20(50)	0(40)	0(40)	-10(40)
C(5)	50(60)	30(50)	20(50)	0(40)	-10(40)	0(40)
C(6)	30(50)	20(40)	20(50)	0(40)	0(40)	0(40)
C(7)	20(40)	20(40)	20(40)	0(30)	0(30)	0(30)
C(8)	20(40)	20(40)	20(40)	0(30)	0(30)	0(30)
C(9)	20(40)	10(40)	20(40)	0(30)	0(30)	0(30)
C(10)	20(40)	20(40)	20(50)	0(40)	0(30)	10(30)
C(11)	20(40)	40(50)	20(50)	-10(40)	0(30)	0(40)
C(12)	20(50)	40(50)	30(60)	-10(40)	-10(40)	0(40)
C(13)	20(50)	30(50)	40(60)	0(40)	0(40)	0(40)
C(14)	20(50)	30(50)	30(50)	0(40)	10(40)	0(40)
C(15)	30(50)	20(40)	20(50)	0(40)	0(40)	0(40)
C(16)	20(40)	20(40)	20(40)	0(40)	0(40)	10(30)
C(17)	30(50)	30(50)	30(50)	10(40)	0(40)	0(40)
C(18)	40(50)	50(60)	30(60)	20(50)	0(40)	20(50)
C(19)	50(60)	30(50)	30(60)	10(40)	10(40)	20(50)
C(20)	50(60)	20(40)	30(50)	0(40)	10(40)	10(40)
C(21)	40(50)	20(50)	20(50)	0(40)	0(40)	10(40)
C(22)	20(40)	10(40)	20(50)	0(30)	0(30)	0(30)
C(23)	20(40)	20(40)	20(50)	0(40)	0(30)	0(30)
C(24)	30(40)	20(40)	30(50)	0(40)	0(40)	0(30)
C(25)	20(40)	20(40)	40(60)	0(40)	0(40)	0(30)
C(26)	20(40)	20(50)	20(50)	10(40)	0(30)	0(30)
C(27)	20(40)	20(40)	20(50)	0(30)	0(30)	0(30)
C(28)	20(40)	20(40)	10(40)	0(30)	0(30)	0(30)
C(29)	20(40)	20(40)	20(50)	0(40)	0(30)	0(30)
C(30)	30(50)	10(40)	30(50)	0(40)	-10(40)	0(30)
C(31)	30(50)	20(40)	30(50)	10(40)	-10(40)	-10(40)
C(32)	20(40)	30(50)	40(60)	0(40)	0(40)	0(40)
C(33)	20(40)	20(40)	20(50)	0(40)	0(40)	0(30)
C(34)	20(40)	20(40)	20(50)	0(40)	0(30)	0(30)
C(35)	30(50)	20(40)	20(50)	0(40)	0(40)	0(40)
C(36)	50(60)	30(50)	30(50)	10(40)	0(40)	0(40)
C(37)	50(60)	20(40)	40(60)	0(50)	10(50)	-10(40)
C(38)	40(50)	20(50)	40(60)	-10(40)	0(40)	-10(40)
C(39)	30(50)	20(50)	20(50)	0(40)	0(40)	0(40)
C(40)	20(40)	20(40)	20(50)	-10(40)	0(30)	0(30)
C(41)	30(50)	30(50)	40(60)	10(40)	0(40)	0(40)
C(42)	20(50)	50(60)	50(70)	10(50)	10(40)	-10(40)
C(43)	20(40)	40(50)	40(60)	-10(50)	0(40)	0(40)
C(44)	30(50)	30(50)	30(50)	-10(40)	0(40)	0(40)
C(45)	20(40)	20(40)	30(50)	0(40)	0(40)	0(30)
C(46)	20(40)	30(50)	20(40)	-10(40)	10(30)	0(40)
C(47)	30(50)	30(50)	20(50)	0(40)	10(40)	0(40)

C(48)	30(50)	50(60)	20(50)	0(40)	0(40)	0(40)
C(49)	30(50)	50(60)	30(60)	0(50)	10(40)	-20(50)
C(50)	40(50)	40(50)	30(60)	0(40)	10(40)	-20(40)
C(51)	30(50)	30(50)	20(50)	0(40)	0(40)	-10(40)
C(52)	30(50)	30(50)	10(40)	0(40)	0(40)	0(40)
C(53)	30(50)	30(50)	20(50)	0(40)	10(40)	0(40)
C(54)	30(50)	50(60)	30(60)	0(50)	0(40)	0(50)
C(55)	30(60)	50(70)	30(60)	10(50)	10(40)	10(50)
C(56)	50(60)	30(50)	30(50)	0(40)	10(40)	10(50)
C(57)	30(50)	30(50)	20(50)	0(40)	0(40)	0(40)
C(58)	30(50)	20(40)	20(50)	0(30)	0(40)	0(40)
C(59)	40(60)	30(50)	20(50)	0(40)	0(40)	10(40)
C(60)	60(70)	30(50)	20(50)	0(40)	0(50)	10(50)
C(61)	70(70)	30(50)	20(50)	0(40)	0(50)	-10(50)
C(62)	60(60)	30(60)	20(50)	0(40)	10(50)	-10(50)
C(63)	40(50)	30(50)	20(50)	0(40)	10(40)	0(40)

Table 54. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for 12· $C_{9.95}$.

	x	y	z	U(eq)
H(2)	9282	7498	8031	24
H(3)	9303	7680	8710	30
H(4)	9868	6843	9123	41
H(5)	10436	5829	8839	41
H(6)	10434	5657	8159	29
H(7A)	9688	7524	7291	22
H(7B)	9009	7131	7429	22
H(8A)	9057	5592	7466	20
H(8B)	9689	5227	7680	20
H(9A)	10902	5985	7493	21
H(9B)	10884	6877	7532	21
H(11)	8584	5834	6246	31
H(12)	7529	5299	6181	39
H(13)	6714	5515	6661	38
H(14)	6965	6262	7208	34
H(15)	8025	6794	7278	26
H(17)	8177	7367	6246	36
H(18)	7927	8493	5933	48
H(19)	8612	9535	6016	44
H(20)	9557	9443	6421	38
H(21)	9795	8328	6752	32
H(23)	10805	4449	6514	24
H(24)	11759	3717	6607	29
H(25)	12096	3390	7246	29
H(26)	11444	3736	7787	27
H(27)	10469	4429	7697	23
H(29)	9798	3474	6780	25
H(30)	8999	2541	6683	30
H(31)	7870	2802	6783	33
H(32)	7541	3993	6994	36
H(33)	8339	4932	7101	26
H(35)	10806	7362	6161	30
H(36)	11000	8591	5959	42
H(37)	11194	9518	6435	43
H(38)	11217	9205	7106	39
H(39)	11075	7963	7305	31
H(41)	12045	7127	6462	40
H(42)	13168	6814	6434	47
H(43)	13570	5756	6764	38
H(44)	12826	5020	7126	34
H(45)	11699	5330	7159	27
H(47)	9063	5847	5229	32
H(48)	8110	5178	5048	40
H(49)	7808	4095	5395	45
H(50)	8454	3690	5930	42
H(51)	9403	4362	6114	33
H(53)	11428	5952	5971	36
H(54)	12389	5214	5966	45
H(55)	12331	3963	5768	48
H(56)	11311	3451	5573	45
H(57)	10337	4179	5584	31
H(59)	9555	7201	5866	38
H(60)	9557	8204	5422	46

H(61)	10116	8106	4820	50
H(62)	10660	6992	4652	46
H(63)	10648	5975	5093	37

Figure 10. Fully-labeled displacement ellipsoid (50%) representation of $[PhB(CH_2PPh_2)_3]Ni(CN^tBu)$ (**13**) (hydrogens omitted for clarity).

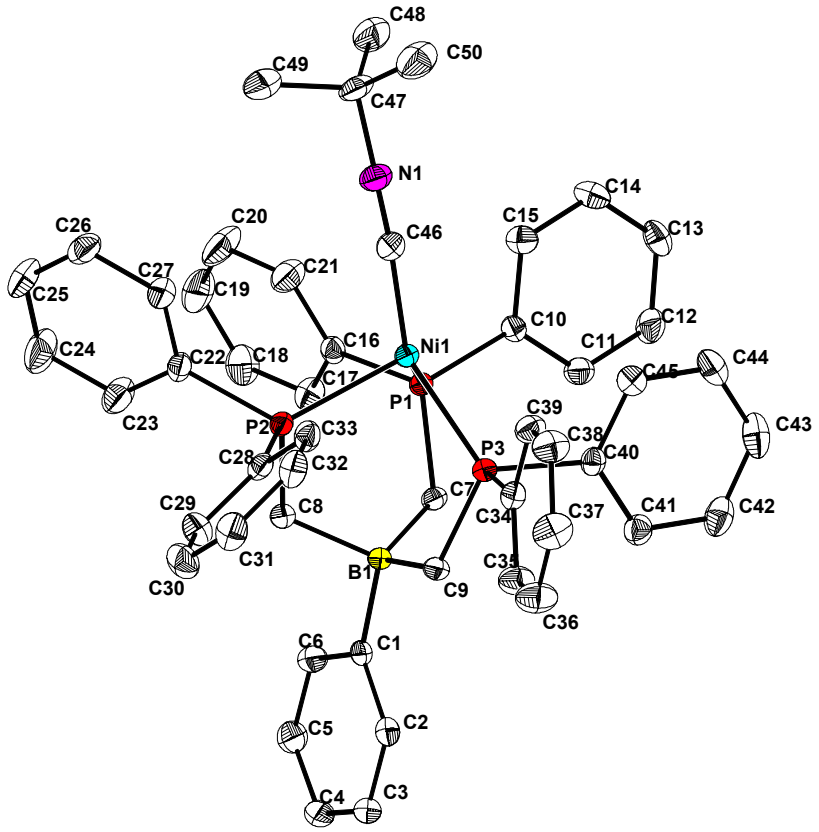


Table 55. Crystal data and structure refinement for 13.

Empirical formula	$C_{50}H_{50}BNNiP_3$	
Moiety formula	$C_{50}H_{50}BNNiP_3$	
Formula weight	827.34	
Crystal habit	rough	
Crystal color	orange	
Crystal size	0.21 x 0.27 x 0.38 mm^3	
Data Collection		
Type of diffractometer	CCD area detector	
Wavelength	0.71073 Å	
Temperature	96(2) K	
Unit cell dimensions	a = 12.3572(10) Å	α = 75.7750(10)°
	b = 13.6104(11) Å	β = 70.8240(10)°
	c = 15.1576(12) Å	γ = 66.4090(10)°
Volume	2187.3(3) $Å^3$	
Z	2	
Crystal system	Triclinic	
Space group	P-1	
Density (calculated)	1.256 g/cm^3	
F(000)	870	
θ range for data collection	1.43 to 28.57°	
Completeness to θ = 28.57°	91.9%	
Index ranges	$-16 \le h \le 16$, $-18 \le k \le 18$, $-20 \le l \le 19$	
Reflections collected	46088	
Independent reflections	10279 [R(int) = 0.0682]	
Absorption coefficient	0.588 mm^{-1}	
Absorption correction	None	
Structure solution and refinement		
Structure solution program	SHELXS-97 (Sheldrick, 1990)	
Primary solution method	direct methods	
Secondary solution method	diffrence Fourier Map	
Hydrogen placement	calculated positions	
Structure refinement program	SHELXL-97 (Sheldrick, 1997)	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	10279 / 0 / 508	
Goodness-of-fit on F^2	1.544	
Final R indices [$I>2\sigma(I)$]	R1 = 0.0411, wR2 = 0.0670	
R indices (all data)	R1 = 0.0700, wR2 = 0.0708	
Type of weighting scheme used	calc	
Weighting scheme used	$w=1/[\sigma^2(F_o^2)]$	
Max shift/error	0.001	
Average shift/error	0.000	
Largest diff. peak and hole	0.926 and -0.432 $e \cdot Å^{-3}$	

Table 56. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (Å^2 x 10^3) for 13. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
Ni(1)	8235(1)	6909(1)	1920(1)	16(1)
P(1)	7123(1)	8662(1)	1717(1)	15(1)
P(2)	7312(1)	6762(1)	3445(1)	16(1)
P(3)	7002(1)	6350(1)	1511(1)	16(1)
N(1)	10944(2)	6038(1)	1764(1)	24(1)
B(1)	5097(2)	7918(2)	2745(2)	16(1)
C(1)	3626(2)	8419(2)	3187(1)	17(1)
C(2)	2792(2)	7967(2)	3194(1)	21(1)
C(3)	1552(2)	8395(2)	3611(1)	25(1)
C(4)	1092(2)	9311(2)	4044(2)	28(1)
C(5)	1888(2)	9784(2)	4052(2)	28(1)
C(6)	3118(2)	9344(2)	3637(1)	23(1)
C(7)	5532(2)	8849(2)	1921(1)	16(1)
C(8)	5723(2)	7632(2)	3646(1)	18(1)
C(9)	5471(2)	6811(2)	2276(1)	17(1)
C(10)	7637(2)	9322(2)	535(1)	16(1)
C(11)	6874(2)	9891(2)	-59(1)	23(1)
C(12)	7335(2)	10318(2)	-968(2)	28(1)
C(13)	8552(2)	10184(2)	-1299(2)	26(1)
C(14)	9320(2)	9630(2)	-712(2)	26(1)
C(15)	8866(2)	9197(2)	186(1)	22(1)
C(16)	7154(2)	9522(2)	2462(1)	18(1)
C(17)	6171(2)	10433(2)	2765(1)	26(1)
C(18)	6251(2)	11053(2)	3322(2)	32(1)
C(19)	7312(2)	10782(2)	3576(2)	38(1)
C(20)	8295(2)	9898(2)	3271(2)	43(1)
C(21)	8212(2)	9264(2)	2725(2)	30(1)
C(22)	7914(2)	6972(2)	4311(1)	18(1)
C(23)	7205(2)	7669(2)	4975(2)	32(1)
C(24)	7698(2)	7774(2)	5636(2)	41(1)
C(25)	8898(2)	7195(2)	5630(2)	35(1)
C(26)	9617(2)	6509(2)	4971(2)	28(1)
C(27)	9126(2)	6398(2)	4316(1)	24(1)
C(28)	7318(2)	5383(2)	3906(1)	18(1)
C(29)	6546(2)	5158(2)	4767(2)	25(1)
C(30)	6560(2)	4111(2)	5099(2)	30(1)
C(31)	7336(2)	3283(2)	4573(2)	29(1)
C(32)	8110(2)	3495(2)	3726(2)	27(1)
C(33)	8105(2)	4546(2)	3397(1)	21(1)
C(34)	7277(2)	4948(2)	1407(1)	19(1)
C(35)	6333(2)	4541(2)	1663(2)	26(1)
C(36)	6571(2)	3471(2)	1598(2)	33(1)
C(37)	7743(2)	2802(2)	1275(2)	31(1)
C(38)	8697(2)	3190(2)	1006(2)	28(1)
C(39)	8457(2)	4256(2)	1079(1)	23(1)
C(40)	6910(2)	6993(2)	308(1)	17(1)
C(41)	5840(2)	7457(2)	15(1)	23(1)
C(42)	5854(2)	7950(2)	-904(2)	30(1)
C(43)	6933(2)	7988(2)	-1538(2)	35(1)
C(44)	8008(2)	7521(2)	-1262(2)	33(1)
C(45)	7989(2)	7034(2)	-347(1)	25(1)
C(46)	9912(2)	6340(2)	1800(1)	20(1)
C(47)	12219(2)	5789(2)	1718(2)	26(1)

C(48)	12501(2)	6820(2)	1310(2)	39(1)
C(49)	12381(2)	5392(2)	2711(2)	35(1)
C(50)	12990(2)	4929(2)	1070(2)	43(1)

Table 57. Selected bond lengths [Å] and angles [°] for 13.

Ni(1)-C(46)	1.861(2)
Ni(1)-P(2)	2.2155(6)
Ni(1)-P(1)	2.2291(6)
Ni(1)-P(3)	2.2515(6)
C(46)-Ni(1)-P(2)	107.38(6)
C(46)-Ni(1)-P(1)	125.59(6)
P(2)-Ni(1)-P(1)	91.86(2)
C(46)-Ni(1)-P(3)	131.77(6)
P(2)-Ni(1)-P(3)	94.58(2)
P(1)-Ni(1)-P(3)	95.00(2)

Table 58. Bond lengths [Å] and angles [°] for 13.

Ni(1)-C(46)	1.861(2)	C(20)-C(21)	1.384(3)
Ni(1)-P(2)	2.2155(6)	C(20)-H(20)	0.9500
Ni(1)-P(1)	2.2291(6)	C(21)-H(21)	0.9500
Ni(1)-P(3)	2.2515(6)	C(22)-C(23)	1.379(3)
P(1)-C(7)	1.8064(19)	C(22)-C(27)	1.386(3)
P(1)-C(10)	1.827(2)	C(23)-C(24)	1.393(3)
P(1)-C(16)	1.8343(19)	C(23)-H(23)	0.9500
P(2)-C(8)	1.8092(19)	C(24)-C(25)	1.372(3)
P(2)-C(28)	1.832(2)	C(24)-H(24)	0.9500
P(2)-C(22)	1.8313(19)	C(25)-C(26)	1.367(3)
P(3)-C(9)	1.8115(19)	C(25)-H(25)	0.9500
P(3)-C(34)	1.837(2)	C(26)-C(27)	1.387(3)
P(3)-C(40)	1.837(2)	C(26)-H(26)	0.9500
N(1)-C(46)	1.159(2)	C(27)-H(27)	0.9500
N(1)-C(47)	1.455(3)	C(28)-C(33)	1.376(3)
B(1)-C(1)	1.629(3)	C(28)-C(29)	1.388(3)
B(1)-C(9)	1.657(3)	C(29)-C(30)	1.385(3)
B(1)-C(8)	1.676(3)	C(29)-H(29)	0.9500
B(1)-C(7)	1.668(3)	C(30)-C(31)	1.378(3)
C(1)-C(2)	1.392(3)	C(30)-H(30)	0.9500
C(1)-C(6)	1.397(3)	C(31)-C(32)	1.371(3)
C(2)-C(3)	1.385(3)	C(31)-H(31)	0.9500
C(2)-H(2)	0.9500	C(32)-C(33)	1.392(3)
C(3)-C(4)	1.378(3)	C(32)-H(32)	0.9500
C(3)-H(3)	0.9500	C(33)-H(33)	0.9500
C(4)-C(5)	1.380(3)	C(34)-C(39)	1.384(3)
C(4)-H(4)	0.9500	C(34)-C(35)	1.390(3)
C(5)-C(6)	1.376(3)	C(35)-C(36)	1.388(3)
C(5)-H(5)	0.9500	C(35)-H(35)	0.9500
C(6)-H(6)	0.9500	C(36)-C(37)	1.365(3)
C(7)-H(7A)	0.9900	C(36)-H(36)	0.9500
C(7)-H(7B)	0.9900	C(37)-C(38)	1.382(3)
C(8)-H(8A)	0.9900	C(37)-H(37)	0.9500
C(8)-H(8B)	0.9900	C(38)-C(39)	1.385(3)
C(9)-H(9A)	0.9900	C(38)-H(38)	0.9500
C(9)-H(9B)	0.9900	C(39)-H(39)	0.9500
C(10)-C(11)	1.389(3)	C(40)-C(41)	1.387(3)
C(10)-C(15)	1.387(3)	C(40)-C(45)	1.388(3)
C(11)-C(12)	1.385(3)	C(41)-C(42)	1.387(3)
C(11)-H(11)	0.9500	C(41)-H(41)	0.9500
C(12)-C(13)	1.370(3)	C(42)-C(43)	1.375(3)
C(12)-H(12)	0.9500	C(42)-H(42)	0.9500
C(13)-C(14)	1.383(3)	C(43)-C(44)	1.380(3)
C(13)-H(13)	0.9500	C(43)-H(43)	0.9500
C(14)-C(15)	1.372(3)	C(44)-C(45)	1.380(3)
C(14)-H(14)	0.9500	C(44)-H(44)	0.9500
C(15)-H(15)	0.9500	C(45)-H(45)	0.9500
C(16)-C(21)	1.378(3)	C(47)-C(48)	1.515(3)
C(16)-C(17)	1.390(3)	C(47)-C(50)	1.516(3)
C(17)-C(18)	1.380(3)	C(47)-C(49)	1.519(3)
C(17)-H(17)	0.9500	C(48)-H(48A)	0.9800
C(18)-C(19)	1.370(3)	C(48)-H(48B)	0.9800
C(18)-H(18)	0.9500	C(48)-H(48C)	0.9800
C(19)-C(20)	1.369(3)	C(49)-H(49A)	0.9800
C(19)-H(19)	0.9500	C(49)-H(49B)	0.9800

C(49)-H(49C)	0.9800	H(7A)-C(7)-H(7B)	107.8
C(50)-H(50A)	0.9800	B(1)-C(8)-P(2)	115.95(13)
C(50)-H(50B)	0.9800	B(1)-C(8)-H(8A)	108.3
C(50)-H(50C)	0.9800	P(2)-C(8)-H(8A)	108.3
C(46)-Ni(1)-P(2)	107.38(6)	B(1)-C(8)-H(8B)	108.3
C(46)-Ni(1)-P(1)	125.59(6)	P(2)-C(8)-H(8B)	108.3
P(2)-Ni(1)-P(1)	91.86(2)	H(8A)-C(8)-H(8B)	107.4
C(46)-Ni(1)-P(3)	131.77(6)	B(1)-C(9)-P(3)	115.85(13)
P(2)-Ni(1)-P(3)	94.58(2)	B(1)-C(9)-H(9A)	108.3
P(1)-Ni(1)-P(3)	95.00(2)	P(3)-C(9)-H(9A)	108.3
C(7)-P(1)-C(10)	108.36(9)	B(1)-C(9)-H(9B)	108.3
C(7)-P(1)-C(16)	105.99(9)	P(3)-C(9)-H(9B)	108.3
C(10)-P(1)-C(16)	101.90(9)	H(9A)-C(9)-H(9B)	107.4
C(7)-P(1)-Ni(1)	110.63(7)	C(11)-C(10)-C(15)	117.89(18)
C(10)-P(1)-Ni(1)	112.52(6)	C(11)-C(10)-P(1)	123.31(15)
C(16)-P(1)-Ni(1)	116.78(7)	C(15)-C(10)-P(1)	118.68(14)
C(8)-P(2)-C(28)	106.33(9)	C(10)-C(11)-C(12)	120.6(2)
C(8)-P(2)-C(22)	106.88(9)	C(10)-C(11)-H(11)	119.7
C(28)-P(2)-C(22)	99.51(9)	C(12)-C(11)-H(11)	119.7
C(8)-P(2)-Ni(1)	110.08(6)	C(13)-C(12)-C(11)	120.58(19)
C(28)-P(2)-Ni(1)	111.43(7)	C(13)-C(12)-H(12)	119.7
C(22)-P(2)-Ni(1)	121.32(7)	C(11)-C(12)-H(12)	119.7
C(9)-P(3)-C(34)	104.50(9)	C(12)-C(13)-C(14)	119.4(2)
C(9)-P(3)-C(40)	107.18(9)	C(12)-C(13)-H(13)	120.3
C(34)-P(3)-C(40)	100.09(8)	C(14)-C(13)-H(13)	120.3
C(9)-P(3)-Ni(1)	109.67(6)	C(15)-C(14)-C(13)	120.0(2)
C(34)-P(3)-Ni(1)	125.87(7)	C(15)-C(14)-H(14)	120.0
C(40)-P(3)-Ni(1)	108.05(6)	C(13)-C(14)-H(14)	120.0
C(46)-N(1)-C(47)	173.4(2)	C(14)-C(15)-C(10)	121.52(19)
C(1)-B(1)-C(9)	110.92(16)	C(14)-C(15)-H(15)	119.2
C(1)-B(1)-C(8)	105.81(15)	C(10)-C(15)-H(15)	119.2
C(9)-B(1)-C(8)	110.60(16)	C(21)-C(16)-C(17)	118.09(19)
C(1)-B(1)-C(7)	108.51(16)	C(21)-C(16)-P(1)	118.48(16)
C(9)-B(1)-C(7)	109.79(16)	C(17)-C(16)-P(1)	123.43(15)
C(8)-B(1)-C(7)	111.14(15)	C(18)-C(17)-C(16)	120.8(2)
C(2)-C(1)-C(6)	114.90(18)	C(18)-C(17)-H(17)	119.6
C(2)-C(1)-B(1)	124.83(17)	C(16)-C(17)-H(17)	119.6
C(6)-C(1)-B(1)	120.21(17)	C(19)-C(18)-C(17)	120.2(2)
C(3)-C(2)-C(1)	123.02(19)	C(19)-C(18)-H(18)	119.9
C(3)-C(2)-H(2)	118.5	C(17)-C(18)-H(18)	119.9
C(1)-C(2)-H(2)	118.5	C(20)-C(19)-C(18)	119.8(2)
C(4)-C(3)-C(2)	120.1(2)	C(20)-C(19)-H(19)	120.1
C(4)-C(3)-H(3)	120.0	C(18)-C(19)-H(19)	120.1
C(2)-C(3)-H(3)	120.0	C(19)-C(20)-C(21)	120.2(2)
C(3)-C(4)-C(5)	118.7(2)	C(19)-C(20)-H(20)	119.9
C(3)-C(4)-H(4)	120.6	C(21)-C(20)-H(20)	119.9
C(5)-C(4)-H(4)	120.6	C(16)-C(21)-C(20)	120.9(2)
C(6)-C(5)-C(4)	120.3(2)	C(16)-C(21)-H(21)	119.6
C(6)-C(5)-H(5)	119.8	C(20)-C(21)-H(21)	119.6
C(4)-C(5)-H(5)	119.8	C(23)-C(22)-C(27)	118.18(18)
C(5)-C(6)-C(1)	122.99(19)	C(23)-C(22)-P(2)	122.74(16)
C(5)-C(6)-H(6)	118.5	C(27)-C(22)-P(2)	119.07(15)
C(1)-C(6)-H(6)	118.5	C(22)-C(23)-C(24)	120.5(2)
B(1)-C(7)-P(1)	113.13(13)	C(22)-C(23)-H(23)	119.8
B(1)-C(7)-H(7A)	109.0	C(24)-C(23)-H(23)	119.8
P(1)-C(7)-H(7A)	109.0	C(25)-C(24)-C(23)	120.4(2)
B(1)-C(7)-H(7B)	109.0	C(25)-C(24)-H(24)	119.8
P(1)-C(7)-H(7B)	109.0	C(23)-C(24)-H(24)	119.8

C(26)-C(25)-C(24)	119.9(2)	C(38)-C(39)-H(39)	119.3
C(26)-C(25)-H(25)	120.1	C(41)-C(40)-C(45)	117.92(19)
C(24)-C(25)-H(25)	120.1	C(41)-C(40)-P(3)	124.72(16)
C(25)-C(26)-C(27)	119.8(2)	C(45)-C(40)-P(3)	117.35(15)
C(25)-C(26)-H(26)	120.1	C(42)-C(41)-C(40)	120.7(2)
C(27)-C(26)-H(26)	120.1	C(42)-C(41)-H(41)	119.7
C(26)-C(27)-C(22)	121.3(2)	C(40)-C(41)-H(41)	119.7
C(26)-C(27)-H(27)	119.4	C(43)-C(42)-C(41)	120.3(2)
C(22)-C(27)-H(27)	119.4	C(43)-C(42)-H(42)	119.8
C(33)-C(28)-C(29)	118.74(19)	C(41)-C(42)-H(42)	119.8
C(33)-C(28)-P(2)	119.85(16)	C(42)-C(43)-C(44)	119.8(2)
C(29)-C(28)-P(2)	121.41(16)	C(42)-C(43)-H(43)	120.1
C(30)-C(29)-C(28)	120.4(2)	C(44)-C(43)-H(43)	120.1
C(30)-C(29)-H(29)	119.8	C(43)-C(44)-C(45)	119.6(2)
C(28)-C(29)-H(29)	119.8	C(43)-C(44)-H(44)	120.2
C(31)-C(30)-C(29)	120.2(2)	C(45)-C(44)-H(44)	120.2
C(31)-C(30)-H(30)	119.9	C(44)-C(45)-C(40)	121.6(2)
C(29)-C(30)-H(30)	119.9	C(44)-C(45)-H(45)	119.2
C(32)-C(31)-C(30)	119.8(2)	C(40)-C(45)-H(45)	119.2
C(32)-C(31)-H(31)	120.1	N(1)-C(46)-Ni(1)	175.14(18)
C(30)-C(31)-H(31)	120.1	N(1)-C(47)-C(48)	107.29(17)
C(31)-C(32)-C(33)	119.9(2)	N(1)-C(47)-C(50)	107.72(17)
C(31)-C(32)-H(32)	120.0	C(48)-C(47)-C(50)	110.4(2)
C(33)-C(32)-H(32)	120.0	N(1)-C(47)-C(49)	107.98(18)
C(28)-C(33)-C(32)	120.8(2)	C(48)-C(47)-C(49)	111.65(18)
C(28)-C(33)-H(33)	119.6	C(50)-C(47)-C(49)	111.64(19)
C(32)-C(33)-H(33)	119.6	C(47)-C(48)-H(48A)	109.5
C(39)-C(34)-C(35)	117.95(19)	C(47)-C(48)-H(48B)	109.5
C(39)-C(34)-P(3)	119.93(15)	H(48A)-C(48)-H(48B)	109.5
C(35)-C(34)-P(3)	122.11(16)	C(47)-C(48)-H(48C)	109.5
C(36)-C(35)-C(34)	120.8(2)	H(48A)-C(48)-H(48C)	109.5
C(36)-C(35)-H(35)	119.6	H(48B)-C(48)-H(48C)	109.5
C(34)-C(35)-H(35)	119.6	C(47)-C(49)-H(49A)	109.5
C(37)-C(36)-C(35)	120.1(2)	C(47)-C(49)-H(49B)	109.5
C(37)-C(36)-H(36)	119.9	H(49A)-C(49)-H(49B)	109.5
C(35)-C(36)-H(36)	119.9	C(47)-C(49)-H(49C)	109.5
C(36)-C(37)-C(38)	120.2(2)	H(49A)-C(49)-H(49C)	109.5
C(36)-C(37)-H(37)	119.9	H(49B)-C(49)-H(49C)	109.5
C(38)-C(37)-H(37)	119.9	C(47)-C(50)-H(50A)	109.5
C(37)-C(38)-C(39)	119.5(2)	C(47)-C(50)-H(50B)	109.5
C(37)-C(38)-H(38)	120.2	H(50A)-C(50)-H(50B)	109.5
C(39)-C(38)-H(38)	120.2	C(47)-C(50)-H(50C)	109.5
C(34)-C(39)-C(38)	121.4(2)	H(50A)-C(50)-H(50C)	109.5
C(34)-C(39)-H(39)	119.3	H(50B)-C(50)-H(50C)	109.5

Table 59. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for 13. The anisotropic displacement factor exponent takes the form: $-2\pi^2[\ h^2 a^{*2} U^{11} + ... + 2\ h\ k\ a^*\ b^*\ U^{12}]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Ni(1)	16(1)	18(1)	16(1)	-1(1)	-5(1)	-7(1)
P(1)	15(1)	17(1)	15(1)	-1(1)	-5(1)	-7(1)
P(2)	18(1)	18(1)	15(1)	0(1)	-6(1)	-8(1)
P(3)	15(1)	17(1)	16(1)	-2(1)	-4(1)	-6(1)
N(1)	19(1)	28(1)	29(1)	-6(1)	-8(1)	-8(1)
B(1)	14(1)	21(1)	15(1)	-2(1)	-4(1)	-9(1)
C(1)	18(1)	22(1)	11(1)	1(1)	-5(1)	-8(1)
C(2)	22(1)	24(1)	16(1)	-3(1)	-4(1)	-8(1)
C(3)	21(1)	40(1)	19(1)	-5(1)	-3(1)	-17(1)
C(4)	15(1)	43(2)	24(1)	-14(1)	0(1)	-8(1)
C(5)	25(1)	33(1)	26(1)	-12(1)	-4(1)	-8(1)
C(6)	20(1)	28(1)	23(1)	-5(1)	-4(1)	-11(1)
C(7)	15(1)	18(1)	17(1)	-3(1)	-6(1)	-6(1)
C(8)	18(1)	20(1)	16(1)	-1(1)	-5(1)	-10(1)
C(9)	15(1)	21(1)	16(1)	1(1)	-4(1)	-9(1)
C(10)	20(1)	14(1)	15(1)	-3(1)	-3(1)	-8(1)
C(11)	20(1)	26(1)	24(1)	0(1)	-7(1)	-10(1)
C(12)	32(1)	31(1)	21(1)	5(1)	-12(1)	-12(1)
C(13)	33(1)	24(1)	18(1)	1(1)	-2(1)	-13(1)
C(14)	19(1)	24(1)	30(1)	-1(1)	0(1)	-9(1)
C(15)	22(1)	20(1)	25(1)	1(1)	-7(1)	-7(1)
C(16)	22(1)	20(1)	14(1)	0(1)	-4(1)	-11(1)
C(17)	29(1)	27(1)	26(1)	-5(1)	-11(1)	-9(1)
C(18)	36(2)	27(1)	30(1)	-12(1)	-7(1)	-7(1)
C(19)	52(2)	40(2)	37(2)	-16(1)	-17(1)	-19(1)
C(20)	42(2)	48(2)	56(2)	-20(1)	-28(1)	-11(1)
C(21)	25(1)	33(1)	37(1)	-12(1)	-12(1)	-7(1)
C(22)	23(1)	20(1)	15(1)	0(1)	-8(1)	-10(1)
C(23)	25(1)	37(1)	35(1)	-12(1)	-15(1)	-2(1)
C(24)	41(2)	47(2)	40(2)	-24(1)	-18(1)	-4(1)
C(25)	40(2)	39(2)	37(2)	-8(1)	-25(1)	-13(1)
C(26)	25(1)	30(1)	32(1)	1(1)	-16(1)	-10(1)
C(27)	26(1)	27(1)	21(1)	-3(1)	-9(1)	-10(1)
C(28)	21(1)	18(1)	19(1)	2(1)	-11(1)	-9(1)
C(29)	27(1)	24(1)	22(1)	-2(1)	-4(1)	-9(1)
C(30)	36(2)	32(1)	22(1)	4(1)	-4(1)	-19(1)
C(31)	45(2)	22(1)	28(1)	5(1)	-15(1)	-19(1)
C(32)	36(1)	24(1)	23(1)	-4(1)	-13(1)	-9(1)
C(33)	27(1)	23(1)	17(1)	2(1)	-9(1)	-11(1)
C(34)	21(1)	19(1)	17(1)	-1(1)	-8(1)	-7(1)
C(35)	21(1)	24(1)	33(1)	-9(1)	-4(1)	-8(1)
C(36)	28(1)	28(1)	46(2)	-7(1)	-7(1)	-16(1)
C(37)	36(2)	18(1)	42(2)	-6(1)	-12(1)	-11(1)
C(38)	22(1)	23(1)	37(1)	-11(1)	-6(1)	-4(1)
C(39)	21(1)	24(1)	26(1)	-5(1)	-7(1)	-10(1)
C(40)	21(1)	16(1)	17(1)	-4(1)	-6(1)	-7(1)
C(41)	23(1)	24(1)	22(1)	-7(1)	-5(1)	-6(1)
C(42)	34(1)	28(1)	27(1)	-5(1)	-17(1)	-2(1)
C(43)	50(2)	32(1)	18(1)	-2(1)	-11(1)	-9(1)
C(44)	34(1)	41(2)	19(1)	-3(1)	1(1)	-15(1)
C(45)	24(1)	28(1)	22(1)	-4(1)	-6(1)	-9(1)
C(46)	24(1)	18(1)	19(1)	-3(1)	-6(1)	-9(1)

C(47)	14(1)	32(1)	36(1)	-12(1)	-9(1)	-6(1)
C(48)	42(2)	51(2)	39(2)	-3(1)	-14(1)	-28(1)
C(49)	25(1)	42(2)	41(2)	-5(1)	-13(1)	-11(1)
C(50)	27(1)	51(2)	52(2)	-28(1)	-14(1)	1(1)

Table 60. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for 13.

H(2)	3087	7336	2898	25
H(3)	1018	8057	3598	30
H(4)	242	9611	4332	33
H(5)	1586	10417	4346	33
H(6)	3646	9684	3657	27
H(7A)	5021	9574	2114	19
H(7B)	5386	8824	1323	19
H(8A)	5242	7285	4198	21
H(8B)	5647	8321	3811	21
H(9A)	4881	6944	1911	21
H(9B)	5378	6220	2794	21
H(11)	6029	9987	161	27
H(12)	6802	10708	-1366	33
H(13)	8866	10469	-1927	31
H(14)	10161	9550	-930	31
H(15)	9405	8803	578	27
H(17)	5435	10632	2586	31
H(18)	5569	11668	3531	38
H(19)	7365	11206	3962	46
H(20)	9038	9718	3434	52
H(21)	8894	8642	2530	36
H(23)	6374	8079	4980	38
H(24)	7199	8251	6094	49
H(25)	9230	7270	6083	42
H(26)	10450	6110	4963	33
H(27)	9630	5918	3861	29
H(29)	6005	5726	5131	30
H(30)	6033	3963	5691	37
H(31)	7334	2568	4797	35
H(32)	8648	2926	3363	32
H(33)	8653	4686	2814	25
H(35)	5514	5001	1886	31
H(36)	5917	3203	1778	39
H(37)	7904	2069	1234	37
H(38)	9512	2728	773	34
H(39)	9116	4517	901	27
H(41)	5090	7437	447	28
H(42)	5115	8263	-1096	36
H(43)	6937	8334	-2164	42
H(44)	8758	7536	-1700	39
H(45)	8732	6718	-160	30
H(48A)	12362	7066	679	59
H(48B)	13357	6681	1268	59
H(48C)	11968	7380	1719	59
H(49A)	11842	5954	3116	53
H(49B)	13233	5230	2698	53
H(49C)	12171	4737	2958	53
H(50A)	12793	4270	1339	64
H(50B)	13858	4770	1003	64
H(50C)	12819	5192	451	64

Figure 11. Fully-labeled displacement ellipsoid (50%) representation of (0.95)[PhB($CH_2P^iPr_2)_3$]NiPMe_3 · (0.05)[PhB($CH_2P^iPr_2)_3$]Tl (**(0.95)14 · (0.05)[PhB$P^{iPr}{}_3$]Tl**) (hydrogens omitted for clarity).

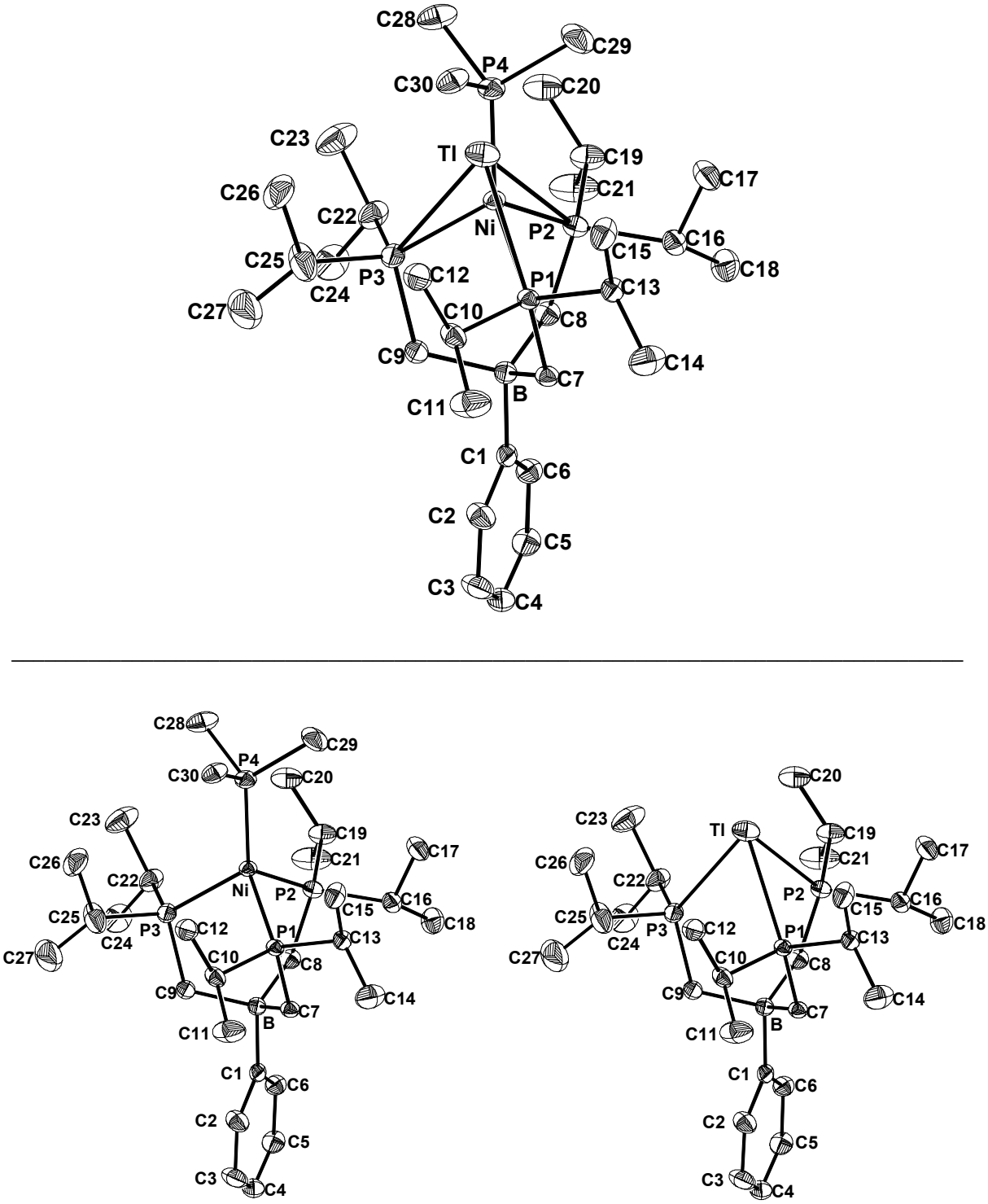


Table 61. Crystal data and structure refinement for (0.95)14 · (0.05)[PhBP$^{iPr}_3$]Tl.

Empirical formula	$C_{29.87}H_{61.60}BNi_{0.95}P_{3.95}Tl_{0.05}$	
Moiety formula	$(0.95)C_{30}H_{62}BNiP_4 \cdot (0.05)C_{27}H_{53}BP_3Tl$	
Formula weight	619.37	
Crystal habit	block	
Crystal color	orange	
Crystal size	0.37 x 0.31 x 0.31 mm^3	
Data Collection		
Type of diffractometer	CCD area detector	
Wavelength	0.71073 Å	
Temperature	100(2) K	
Unit cell dimensions	a = 9.6258(5) Å	α = 90°
	b = 21.6538(12) Å	β = 93.871(2)°
	c = 16.8244(9) Å	γ = 90°
Volume	3498.8(3) Å^3	
Z	4	
Crystal system	Monoclinic	
Space group	$P2_1/c$	
Density (calculated)	1.176 g/cm^3	
F(000)	1342	
θ range for data collection	1.53 to 35.06°	
Completeness to θ = 35.06°	89.0%	
Index ranges	$-15 \le h \le 12$, $-34 \le k \le 28$, $-26 \le l \le 25$	
Reflections collected	67064	
Independent reflections	13791 [R(int) = 0.0656]	
Absorption coefficient	0.935 mm^{-1}	
Absorption correction	None	
Structure solution and refinement		
Structure solution program	SHELXS-97 (Sheldrick, 1990)	
Primary solution method	Direct methods	
Secondary solution method	Difference Fourier map	
Hydrogen placement	Calculated positions	
Structure refinement program	SHELXL-97 (Sheldrick, 1997)	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	13791 / 0 / 350	
Goodness-of-fit on F^2	1.518	
Final R indices [$I>2\sigma(I)$]	R1 = 0.0534, wR2 = 0.0925	
R indices (all data)	R1 = 0.0988, wR2 = 0.0970	
Type of weighting scheme used	Calculated	
Weighting scheme used	$w=1/[\sigma^2(F_o^2)+(0.02P)^2]$ where $P=(F_o^2+2F_c^2)/3$	
Max shift/error	0.001	
Average shift/error	0.000	
Largest diff. peak and hole	1.324 and -0.983 e·Å^{-3}	

Special Refinement Details: The crystal contained <5% of a starting material impurity, identified by the presence of a thallium atom, which was anisotropically refined.

Table 62. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$ x 10^3) for (0.95)14 · (0.05)[PhBP$^{iPr}_3$]Tl. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
P(1)	1847(1)	6074(1)	6713(1)	16(1)
P(2)	1671(1)	6165(1)	8649(1)	19(1)
P(3)	-597(1)	6997(1)	7385(1)	22(1)
B	2472(2)	7211(1)	7642(1)	18(1)
C(1)	3528(2)	7806(1)	7652(1)	19(1)
C(2)	3888(2)	8076(1)	6940(1)	28(1)
C(3)	4722(2)	8597(1)	6911(1)	32(1)
C(4)	5243(2)	8874(1)	7613(1)	28(1)
C(5)	4909(2)	8629(1)	8326(1)	26(1)
C(6)	4062(2)	8105(1)	8343(1)	23(1)
C(7)	3087(2)	6672(1)	7055(1)	18(1)
C(8)	2364(2)	6947(1)	8562(1)	20(1)
C(9)	936(2)	7483(1)	7276(1)	21(1)
C(10)	1205(2)	6362(1)	5711(1)	22(1)
C(11)	2276(2)	6431(1)	5079(1)	44(1)
C(12)	-50(2)	6001(1)	5359(1)	30(1)
C(13)	2915(2)	5368(1)	6563(1)	19(1)
C(14)	4276(2)	5451(1)	6155(1)	42(1)
C(15)	2074(2)	4839(1)	6183(1)	31(1)
C(16)	3279(2)	5678(1)	8773(1)	22(1)
C(17)	2901(2)	4991(1)	8808(1)	32(1)
C(18)	4310(2)	5847(1)	9479(1)	33(1)
C(19)	1017(2)	6082(1)	9677(1)	28(1)
C(20)	-490(2)	5865(1)	9651(1)	36(1)
C(21)	1231(3)	6651(1)	10207(1)	45(1)
C(22)	-1349(2)	7282(1)	8314(1)	30(1)
C(23)	-2814(2)	7025(1)	8402(2)	48(1)
C(24)	-1340(2)	7982(1)	8466(1)	39(1)
C(25)	-1818(2)	7235(1)	6531(2)	54(1)
C(26)	-3040(2)	6804(1)	6358(1)	42(1)
C(27)	-2055(3)	7882(1)	6357(2)	75(1)
Ni	156(1)	6002(1)	7571(1)	16(1)
P(4)	-1281(1)	5174(1)	7487(1)	23(1)
C(28)	-2929(2)	5254(1)	7973(1)	35(1)
C(29)	-668(2)	4435(1)	7912(1)	39(1)
C(30)	-1967(2)	4902(1)	6506(1)	28(1)
Tl	-590(2)	5711(1)	7494(1)	32(1)

Table 63. Selected bond lengths [Å] and angles [°] for (0.95)14 · (0.05)[PhBP$^{iPr}_3$]Tl.

P(1)-Ni	2.2533(5)	P(1)-Ni-P(4)	118.670(19)
P(2)-Ni	2.2764(5)	P(1)-Ni-P(2)	92.761(19)
P(3)-Ni	2.2873(5)	P(4)-Ni-P(2)	121.90(2)
B-Ni	3.4356(18)	P(1)-Ni-P(3)	94.739(18)
Ni-P(4)	2.2631(5)	P(4)-Ni-P(3)	123.43(2)
		P(2)-Ni-P(3)	98.240(19)

Table 64. Bond lengths [Å] and angles [°] for (0.95)14 · (0.05)[PhBP$^{iPr}_3$]Tl.

P(1)-C(7)	1.8278(16)	C(16)-C(18)	1.539(2)
P(1)-C(10)	1.8633(17)	C(16)-H(16)	1.0000
P(1)-C(13)	1.8684(16)	C(17)-H(17A)	0.9800
P(1)-Ni	2.2533(5)	C(17)-H(17B)	0.9800
P(1)-Tl	2.874(2)	C(17)-H(17C)	0.9800
P(2)-C(8)	1.8308(17)	C(18)-H(18A)	0.9800
P(2)-C(16)	1.8722(18)	C(18)-H(18B)	0.9800
P(2)-C(19)	1.8891(18)	C(18)-H(18C)	0.9800
P(2)-Ni	2.2764(5)	C(19)-C(20)	1.523(3)
P(2)-Tl	2.984(2)	C(19)-C(21)	1.526(3)
P(3)-C(9)	1.8320(17)	C(19)-H(19)	1.0000
P(3)-C(25)	1.866(2)	C(20)-H(20A)	0.9800
P(3)-C(22)	1.8719(19)	C(20)-H(20B)	0.9800
P(3)-Ni	2.2873(5)	C(20)-H(20C)	0.9800
P(3)-Tl	2.790(2)	C(21)-H(21A)	0.9800
B-C(1)	1.641(2)	C(21)-H(21B)	0.9800
B-C(8)	1.659(3)	C(21)-H(21C)	0.9800
B-C(7)	1.663(2)	C(22)-C(23)	1.532(3)
B-C(9)	1.671(2)	C(22)-C(24)	1.537(3)
B-Ni	3.4356(18)	C(22)-H(22)	1.0000
C(1)-C(2)	1.398(2)	C(23)-H(23A)	0.9800
C(1)-C(6)	1.398(2)	C(23)-H(23B)	0.9800
C(2)-C(3)	1.387(2)	C(23)-H(23C)	0.9800
C(2)-H(2)	0.9500	C(24)-H(24A)	0.9800
C(3)-C(4)	1.387(3)	C(24)-H(24B)	0.9800
C(3)-H(3)	0.9500	C(24)-H(24C)	0.9800
C(4)-C(5)	1.370(3)	C(25)-C(27)	1.446(3)
C(4)-H(4)	0.9500	C(25)-C(26)	1.514(3)
C(5)-C(6)	1.398(2)	C(25)-H(25)	1.0000
C(5)-H(5)	0.9500	C(26)-H(26A)	0.9800
C(6)-H(6)	0.9500	C(26)-H(26B)	0.9800
C(7)-H(7A)	0.9900	C(26)-H(26C)	0.9800
C(7)-H(7B)	0.9900	C(27)-H(27A)	0.9800
C(8)-H(8A)	0.9900	C(27)-H(27B)	0.9800
C(8)-H(8B)	0.9900	C(27)-H(27C)	0.9800
C(9)-H(9A)	0.9900	Ni-P(4)	2.2631(5)
C(9)-H(9B)	0.9900	P(4)-C(29)	1.834(2)
C(10)-C(12)	1.525(2)	P(4)-C(30)	1.8337(19)
C(10)-C(11)	1.537(3)	P(4)-C(28)	1.841(2)
C(10)-H(10)	1.0000	C(28)-H(28A)	0.9800
C(11)-H(11A)	0.9800	C(28)-H(28B)	0.9800
C(11)-H(11B)	0.9800	C(28)-H(28C)	0.9800
C(11)-H(11C)	0.9800	C(29)-H(29A)	0.9800
C(12)-H(12A)	0.9800	C(29)-H(29B)	0.9800
C(12)-H(12B)	0.9800	C(29)-H(29C)	0.9800
C(12)-H(12C)	0.9800	C(30)-H(30A)	0.9800
C(13)-C(15)	1.520(2)	C(30)-H(30B)	0.9800
C(13)-C(14)	1.531(2)	C(30)-H(30C)	0.9800
C(13)-H(13)	1.0000		
C(14)-H(14A)	0.9800	C(7)-P(1)-C(10)	102.59(8)
C(14)-H(14B)	0.9800	C(7)-P(1)-C(13)	105.54(8)
C(14)-H(14C)	0.9800	C(10)-P(1)-C(13)	107.70(8)
C(15)-H(15A)	0.9800	C(7)-P(1)-Ni	109.37(5)
C(15)-H(15B)	0.9800	C(10)-P(1)-Ni	113.17(6)
C(15)-H(15C)	0.9800	C(13)-P(1)-Ni	117.22(6)
C(16)-C(17)	1.534(2)	C(7)-P(1)-Tl	125.82(7)

C(10)-P(1)-Tl	105.92(7)	B-C(8)-H(8A)	108.3
C(13)-P(1)-Tl	108.14(7)	P(2)-C(8)-H(8A)	108.3
Ni-P(1)-Tl	16.45(4)	B-C(8)-H(8B)	108.3
C(8)-P(2)-C(16)	103.10(8)	P(2)-C(8)-H(8B)	108.3
C(8)-P(2)-C(19)	107.88(8)	H(8A)-C(8)-H(8B)	107.4
C(16)-P(2)-C(19)	99.70(8)	B-C(9)-P(3)	117.32(11)
C(8)-P(2)-Ni	107.27(6)	B-C(9)-H(9A)	108.0
C(16)-P(2)-Ni	118.83(6)	P(3)-C(9)-H(9A)	108.0
C(19)-P(2)-Ni	118.65(6)	B-C(9)-H(9B)	108.0
C(8)-P(2)-Tl	120.41(7)	P(3)-C(9)-H(9B)	108.0
C(16)-P(2)-Tl	116.66(7)	H(9A)-C(9)-H(9B)	107.2
C(19)-P(2)-Tl	106.96(7)	C(12)-C(10)-C(11)	109.41(15)
Ni-P(2)-Tl	14.19(4)	C(12)-C(10)-P(1)	112.66(12)
C(9)-P(3)-C(25)	103.52(9)	C(11)-C(10)-P(1)	117.44(13)
C(9)-P(3)-C(22)	104.66(8)	C(12)-C(10)-H(10)	105.4
C(25)-P(3)-C(22)	106.98(11)	C(11)-C(10)-H(10)	105.4
C(9)-P(3)-Ni	107.79(6)	P(1)-C(10)-H(10)	105.4
C(25)-P(3)-Ni	122.91(7)	C(10)-C(11)-H(11A)	109.5
C(22)-P(3)-Ni	109.46(6)	C(10)-C(11)-H(11B)	109.5
C(9)-P(3)-Tl	125.60(7)	H(11A)-C(11)-H(11B)	109.5
C(25)-P(3)-Tl	108.98(8)	C(10)-C(11)-H(11C)	109.5
C(22)-P(3)-Tl	105.89(7)	H(11A)-C(11)-H(11C)	109.5
Ni-P(3)-Tl	18.56(4)	H(11B)-C(11)-H(11C)	109.5
C(1)-B-C(8)	109.80(14)	C(10)-C(12)-H(12A)	109.5
C(1)-B-C(7)	108.19(13)	C(10)-C(12)-H(12B)	109.5
C(8)-B-C(7)	111.06(13)	H(12A)-C(12)-H(12B)	109.5
C(1)-B-C(9)	105.00(13)	C(10)-C(12)-H(12C)	109.5
C(8)-B-C(9)	110.82(14)	H(12A)-C(12)-H(12C)	109.5
C(7)-B-C(9)	111.76(14)	H(12B)-C(12)-H(12C)	109.5
C(1)-B-Ni	177.48(12)	C(15)-C(13)-C(14)	110.30(15)
C(8)-B-Ni	71.87(8)	C(15)-C(13)-P(1)	113.03(12)
C(7)-B-Ni	72.59(8)	C(14)-C(13)-P(1)	117.43(12)
C(9)-B-Ni	72.53(8)	C(15)-C(13)-H(13)	104.9
C(2)-C(1)-C(6)	114.84(15)	C(14)-C(13)-H(13)	104.9
C(2)-C(1)-B	120.66(15)	P(1)-C(13)-H(13)	104.9
C(6)-C(1)-B	124.38(15)	C(13)-C(14)-H(14A)	109.5
C(3)-C(2)-C(1)	123.21(17)	C(13)-C(14)-H(14B)	109.5
C(3)-C(2)-H(2)	118.4	H(14A)-C(14)-H(14B)	109.5
C(1)-C(2)-H(2)	118.4	C(13)-C(14)-H(14C)	109.5
C(4)-C(3)-C(2)	119.90(18)	H(14A)-C(14)-H(14C)	109.5
C(4)-C(3)-H(3)	120.1	H(14B)-C(14)-H(14C)	109.5
C(2)-C(3)-H(3)	120.1	C(13)-C(15)-H(15A)	109.5
C(5)-C(4)-C(3)	119.06(16)	C(13)-C(15)-H(15B)	109.5
C(5)-C(4)-H(4)	120.5	H(15A)-C(15)-H(15B)	109.5
C(3)-C(4)-H(4)	120.5	C(13)-C(15)-H(15C)	109.5
C(4)-C(5)-C(6)	120.22(17)	H(15A)-C(15)-H(15C)	109.5
C(4)-C(5)-H(5)	119.9	H(15B)-C(15)-H(15C)	109.5
C(6)-C(5)-H(5)	119.9	C(17)-C(16)-C(18)	110.08(15)
C(5)-C(6)-C(1)	122.77(17)	C(17)-C(16)-P(2)	110.69(12)
C(5)-C(6)-H(6)	118.6	C(18)-C(16)-P(2)	115.94(13)
C(1)-C(6)-H(6)	118.6	C(17)-C(16)-H(16)	106.5
B-C(7)-P(1)	115.66(11)	C(18)-C(16)-H(16)	106.5
B-C(7)-H(7A)	108.4	P(2)-C(16)-H(16)	106.5
P(1)-C(7)-H(7A)	108.4	C(16)-C(17)-H(17A)	109.5
B-C(7)-H(7B)	108.4	C(16)-C(17)-H(17B)	109.5
P(1)-C(7)-H(7B)	108.4	H(17A)-C(17)-H(17B)	109.5
H(7A)-C(7)-H(7B)	107.4	C(16)-C(17)-H(17C)	109.5
B-C(8)-P(2)	116.06(11)	H(17A)-C(17)-H(17C)	109.5

H(17B)-C(17)-H(17C)	109.5	C(22)-C(24)-H(24C)	109.5
C(16)-C(18)-H(18A)	109.5	H(24A)-C(24)-H(24C)	109.5
C(16)-C(18)-H(18B)	109.5	H(24B)-C(24)-H(24C)	109.5
H(18A)-C(18)-H(18B)	109.5	C(27)-C(25)-C(26)	116.64(19)
C(16)-C(18)-H(18C)	109.5	C(27)-C(25)-P(3)	120.42(17)
H(18A)-C(18)-H(18C)	109.5	C(26)-C(25)-P(3)	114.74(16)
H(18B)-C(18)-H(18C)	109.5	C(27)-C(25)-H(25)	99.6
C(20)-C(19)-C(21)	110.95(17)	C(26)-C(25)-H(25)	99.6
C(20)-C(19)-P(2)	112.21(13)	P(3)-C(25)-H(25)	99.6
C(21)-C(19)-P(2)	114.73(13)	C(25)-C(26)-H(26A)	109.5
C(20)-C(19)-H(19)	106.1	C(25)-C(26)-H(26B)	109.5
C(21)-C(19)-H(19)	106.1	H(26A)-C(26)-H(26B)	109.5
P(2)-C(19)-H(19)	106.1	C(25)-C(26)-H(26C)	109.5
C(19)-C(20)-H(20A)	109.5	H(26A)-C(26)-H(26C)	109.5
C(19)-C(20)-H(20B)	109.5	H(26B)-C(26)-H(26C)	109.5
H(20A)-C(20)-H(20B)	109.5	C(25)-C(27)-H(27A)	109.5
C(19)-C(20)-H(20C)	109.5	C(25)-C(27)-H(27B)	109.5
H(20A)-C(20)-H(20C)	109.5	H(27A)-C(27)-H(27B)	109.5
H(20B)-C(20)-H(20C)	109.5	C(25)-C(27)-H(27C)	109.5
C(19)-C(21)-H(21A)	109.5	H(27A)-C(27)-H(27C)	109.5
C(19)-C(21)-H(21B)	109.5	H(27B)-C(27)-H(27C)	109.5
H(21A)-C(21)-H(21B)	109.5	P(1)-Ni-P(4)	118.670(19)
C(19)-C(21)-H(21C)	109.5	P(1)-Ni-P(2)	92.761(19)
H(21A)-C(21)-H(21C)	109.5	P(4)-Ni-P(2)	121.90(2)
H(21B)-C(21)-H(21C)	109.5	P(1)-Ni-P(3)	94.739(18)
C(23)-C(22)-C(24)	109.68(16)	P(4)-Ni-P(3)	123.43(2)
C(23)-C(22)-P(3)	111.80(14)	P(2)-Ni-P(3)	98.240(19)
C(24)-C(22)-P(3)	117.78(14)	P(1)-Ni-B	58.28(3)
C(23)-C(22)-H(22)	105.5	P(4)-Ni-B	176.73(4)
C(24)-C(22)-H(22)	105.5	P(2)-Ni-B	58.33(4)
P(3)-C(22)-H(22)	105.5	P(3)-Ni-B	59.07(3)
C(22)-C(23)-H(23A)	109.5	C(29)-P(4)-C(30)	99.09(10)
C(22)-C(23)-H(23B)	109.5	C(29)-P(4)-C(28)	100.02(10)
H(23A)-C(23)-H(23B)	109.5	C(30)-P(4)-C(28)	99.29(9)
C(22)-C(23)-H(23C)	109.5	C(29)-P(4)-Ni	119.19(7)
H(23A)-C(23)-H(23C)	109.5	C(30)-P(4)-Ni	119.46(6)
H(23B)-C(23)-H(23C)	109.5	C(28)-P(4)-Ni	116.02(7)
C(22)-C(24)-H(24A)	109.5	P(3)-Tl-P(1)	72.27(5)
C(22)-C(24)-H(24B)	109.5	P(3)-Tl-P(2)	73.31(5)
H(24A)-C(24)-H(24B)	109.5	P(1)-Tl-P(2)	68.04(5)

Table 65. Anisotropic displacement parameters ($Å^2$x 10^3) for (0.95)14 · (0.05)[$PhBP^{iPr}_3$]Tl. The anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U^{11} + ... + 2 h k a^* b^* U^{12}]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
P(1)	17(1)	13(1)	17(1)	0(1)	1(1)	-2(1)
P(2)	22(1)	17(1)	18(1)	0(1)	3(1)	-3(1)
P(3)	18(1)	15(1)	34(1)	-1(1)	-1(1)	-2(1)
B	18(1)	13(1)	23(1)	-2(1)	-1(1)	-2(1)
C(1)	16(1)	12(1)	29(1)	0(1)	0(1)	1(1)
C(2)	33(1)	21(1)	28(1)	3(1)	-9(1)	-8(1)
C(3)	39(1)	25(1)	31(1)	9(1)	-2(1)	-11(1)
C(4)	25(1)	18(1)	42(1)	3(1)	-4(1)	-8(1)
C(5)	25(1)	19(1)	35(1)	-8(1)	-2(1)	-4(1)
C(6)	22(1)	18(1)	29(1)	-3(1)	4(1)	-1(1)
C(7)	18(1)	17(1)	18(1)	1(1)	-1(1)	-5(1)
C(8)	21(1)	17(1)	23(1)	-4(1)	0(1)	-3(1)
C(9)	19(1)	14(1)	28(1)	0(1)	0(1)	-1(1)
C(10)	28(1)	19(1)	18(1)	3(1)	-4(1)	-3(1)
C(11)	43(1)	65(2)	23(1)	11(1)	-3(1)	-23(1)
C(12)	28(1)	33(1)	27(1)	6(1)	-7(1)	-7(1)
C(13)	20(1)	16(1)	22(1)	-3(1)	1(1)	1(1)
C(14)	35(1)	25(1)	68(2)	-8(1)	21(1)	0(1)
C(15)	25(1)	20(1)	47(1)	-10(1)	-5(1)	3(1)
C(16)	24(1)	22(1)	20(1)	2(1)	1(1)	1(1)
C(17)	38(1)	23(1)	36(1)	7(1)	2(1)	4(1)
C(18)	32(1)	39(1)	27(1)	3(1)	-5(1)	1(1)
C(19)	34(1)	30(1)	19(1)	-3(1)	6(1)	-9(1)
C(20)	41(1)	38(1)	31(1)	-1(1)	12(1)	-11(1)
C(21)	63(2)	48(1)	26(1)	-13(1)	18(1)	-26(1)
C(22)	23(1)	24(1)	44(1)	-7(1)	9(1)	1(1)
C(23)	29(1)	38(1)	78(2)	-21(1)	20(1)	-6(1)
C(24)	37(1)	29(1)	52(1)	-17(1)	3(1)	0(1)
C(25)	48(2)	27(1)	81(2)	13(1)	-36(1)	-9(1)
C(26)	24(1)	42(1)	58(2)	-4(1)	-10(1)	-5(1)
C(27)	55(2)	62(2)	102(2)	40(2)	-37(2)	-16(1)
Ni	16(1)	13(1)	20(1)	-1(1)	2(1)	-2(1)
P(4)	22(1)	16(1)	30(1)	-2(1)	2(1)	-6(1)
C(28)	32(1)	35(1)	40(1)	-12(1)	10(1)	-16(1)
C(29)	46(1)	19(1)	49(1)	6(1)	-8(1)	-9(1)
C(30)	23(1)	27(1)	34(1)	-9(1)	3(1)	-9(1)
Tl	37(1)	23(1)	36(1)	-2(1)	5(1)	-10(1)

Table 66. Hydrogen coordinates (x 10^4) and isotropic displacement parameters (Å^{2}x 10^3) for (0.95)14 · (0.05)[PhBP$^{iPr}_3$]Tl.

	x	y	z	U(eq)
H(2)	3546	7894	6451	33
H(3)	4936	8765	6412	38
H(4)	5822	9228	7599	34
H(5)	5254	8815	8811	31
H(6)	3841	7945	8845	27
H(7A)	3892	6470	7346	21
H(7B)	3436	6877	6582	21
H(8A)	1769	7233	8848	24
H(8B)	3306	6959	8836	24
H(9A)	1004	7566	6701	25
H(9B)	774	7884	7536	25
H(10)	853	6789	5802	27
H(11A)	2498	6023	4870	66
H(11B)	3126	6621	5322	66
H(11C)	1889	6693	4644	66
H(12A)	-477	6224	4898	45
H(12B)	-731	5954	5762	45
H(12C)	252	5592	5190	45
H(13)	3206	5222	7113	23
H(14A)	4851	5080	6237	63
H(14B)	4782	5809	6383	63
H(14C)	4068	5516	5583	63
H(15A)	1892	4919	5613	46
H(15B)	1188	4803	6435	46
H(15C)	2600	4453	6258	46
H(16)	3788	5736	8280	26
H(17A)	3750	4742	8805	48
H(17B)	2276	4884	8344	48
H(17C)	2435	4908	9297	48
H(18A)	3879	5766	9980	50
H(18B)	4550	6286	9450	50
H(18C)	5155	5597	9457	50
H(19)	1584	5745	9945	33
H(20A)	-774	5812	10195	54
H(20B)	-576	5470	9367	54
H(20C)	-1090	6172	9372	54
H(21A)	626	6985	9998	68
H(21B)	2206	6783	10213	68
H(21C)	1000	6549	10750	68
H(22)	-753	7099	8764	36
H(23A)	-3076	7093	8948	71
H(23B)	-2824	6582	8287	71
H(23C)	-3478	7237	8028	71
H(24A)	-1894	8190	8035	59
H(24B)	-380	8135	8485	59
H(24C)	-1740	8067	8975	59
H(25)	-1244	7124	6079	64
H(26A)	-3761	6891	6727	63
H(26B)	-2728	6375	6426	63
H(26C)	-3422	6867	5809	63
H(27A)	-2421	7928	5803	112
H(27B)	-1175	8108	6439	112
H(27C)	-2729	8048	6713	112

H(28A)	-3487	5585	7713	53
H(28B)	-2730	5356	8537	53
H(28C)	-3448	4865	7928	53
H(29A)	-423	4486	8483	58
H(29B)	154	4299	7646	58
H(29C)	-1406	4125	7833	58
H(30A)	-2594	4552	6572	42
H(30B)	-1194	4772	6194	42
H(30C)	-2480	5238	6226	42

Figure 12. Fully-labeled displacement ellipsoid (50%) representation of $[PhB(CH_2P^iPr_2)_3]Ni(CN^tBu)$ (**15**) (hydrogens omitted for clarity).

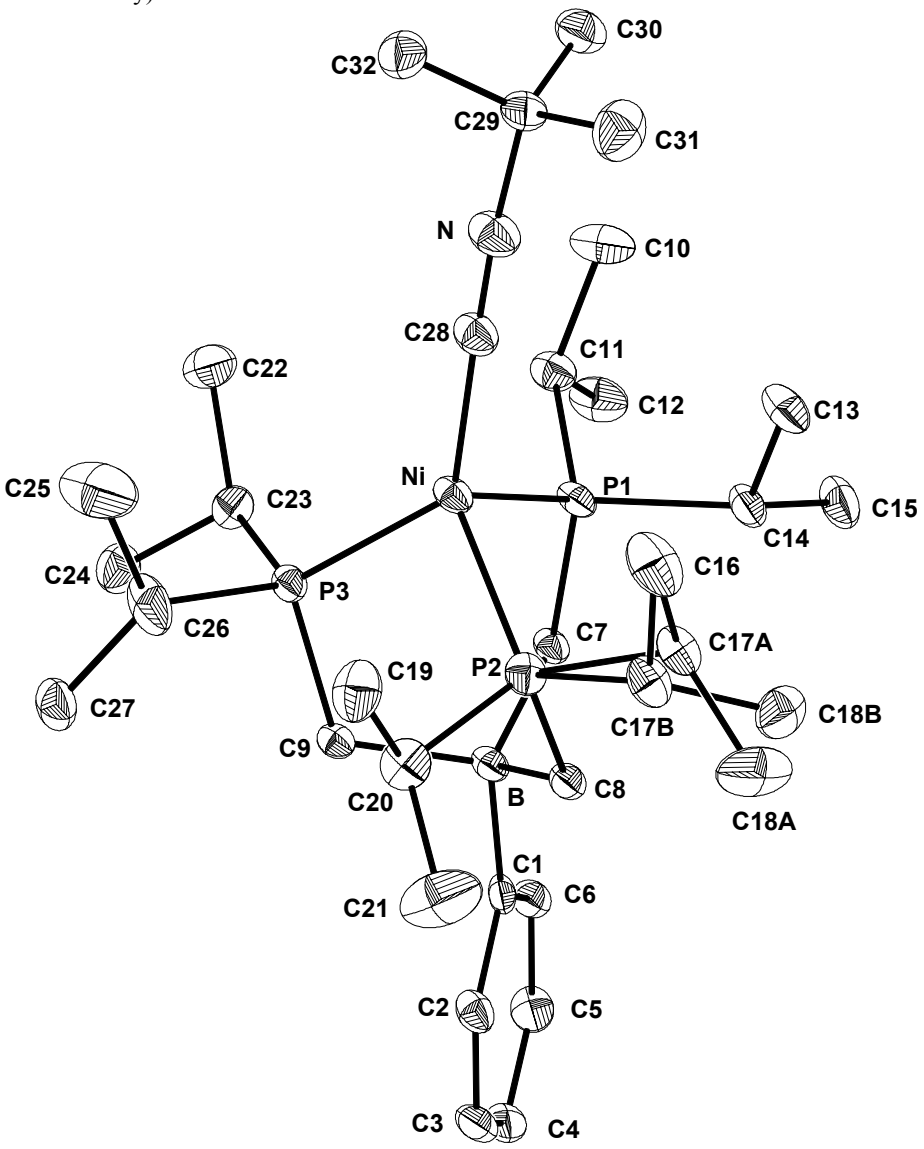


Table 67. Crystal data and structure refinement for 15.

Empirical formula	$C_{32}H_{62}BNNiP_3$	
Moiety formula	$C_{32}H_{62}BNNiP_3$	
Formula weight	623.26	
Crystal habit	plate	
Crystal color	yellow	
Crystal size	0.33 x 0.30 x 0.14 mm^3	
Data Collection		
Type of diffractometer	CCD area detector	
Wavelength	0.71073 Å	
Temperature	100(2) K	
Unit cell dimensions	a = 9.6300(7) Å	α = 87.053(1)°
	b = 12.2632(9) Å	β = 80.119(1)°
	c = 15.4425(11) Å	γ = 84.968(1)°
Volume	1788.5(2) $Å^3$	
Z	2	
Crystal system	Triclinic	
Space group	$P\bar{1}$ (#2)	
Density (calculated)	1.157 g/cm^3	
F(000)	678	
θ range for data collection	1.67 to 28.40°	
Completeness to θ = 28.40°	91.4%	
Index ranges	$-12 \le h \le 12$, $-16 \le k \le 16$, $-20 \le l \le 20$	
Reflections collected	31909	
Independent reflections	8214 [R(int) = 0.0590]	
Absorption coefficient	0.697 mm^{-1}	
Absorption correction	None	
Structure solution and refinement		
Structure solution program	SHELXS-97 (Sheldrick, 1990)	
Primary solution method	Direct methods	
Secondary solution method	Difference Fourier map	
Hydrogen placement	Calculated positions	
Structure refinement program	SHELXL-97 (Sheldrick, 1997)	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	8214 / 0 / 368	
Goodness-of-fit on F^2	1.674	
Final R indices [$I>2\sigma(I)$]	R1 = 0.0410, wR2 = 0.0876	
R indices (all data)	R1 = 0.0557, wR2 = 0.0909	
Type of weighting scheme used	Calculated	
Weighting scheme used	$w=1/[\sigma^2(F_o^2)+(0.02P)^2]$ where $P=(F_o^2+2F_c^2)/3$	
Max shift/error	0.001	
Average shift/error	0.000	
Max. and min. transmission	0.907 and 0.795	
Largest diff. peak and hole	0.886 and -0.621 $e \cdot Å^{-3}$	

Special Refinement Details: One isopropyl group was successfully modeled as disordered over two positions.

Table 68. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$ x 10^3) for 15. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
Ni	1360(1)	2110(1)	2338(1)	17(1)
P(3)	191(1)	3652(1)	2914(1)	17(1)
P(2)	2816(1)	2955(1)	1239(1)	20(1)
P(1)	2845(1)	1953(1)	3315(1)	17(1)
B	3144(2)	4279(2)	2745(1)	17(1)
C(1)	3941(2)	5344(2)	2927(1)	16(1)
C(2)	4129(2)	6223(2)	2311(1)	20(1)
C(3)	4724(2)	7171(2)	2463(1)	23(1)
C(4)	5159(2)	7293(2)	3262(1)	22(1)
C(5)	4989(2)	6453(2)	3894(1)	22(1)
C(6)	4408(2)	5506(2)	3722(1)	19(1)
C(7)	3339(2)	3310(1)	3520(1)	16(1)
C(8)	3868(2)	3817(2)	1753(1)	18(1)
C(9)	1436(2)	4720(2)	2810(1)	15(1)
C(10)	2044(3)	98(2)	4405(2)	33(1)
C(11)	2161(2)	1333(2)	4418(1)	22(1)
C(12)	2900(3)	1610(2)	5177(1)	29(1)
C(13)	4429(2)	133(2)	2457(1)	28(1)
C(14)	4583(2)	1204(2)	2899(1)	21(1)
C(15)	5632(2)	1007(2)	3542(2)	28(1)
C(17A)	4184(9)	1969(8)	598(7)	22(2)
C(18A)	5472(11)	2498(10)	68(8)	53(3)
C(17B)	3976(6)	2244(5)	285(5)	25(1)
C(18B)	5514(5)	2012(6)	405(5)	34(2)
C(16)	3418(3)	1208(2)	80(2)	39(1)
C(19)	932	3399	32	34
C(20)	1882(2)	3953(2)	533(1)	26(1)
C(21)	2808(3)	4723(3)	-81(2)	61(1)
C(22)	-1453(2)	2638(2)	4379(2)	30(1)
C(23)	-568(2)	3612(2)	4110(1)	23(1)
C(24)	-1394(2)	4669(2)	4471(1)	28(1)
C(25)	-2355(3)	3462(2)	2309(2)	76(1)
C(26)	-1263(3)	4193(2)	2312(2)	38(1)
C(27)	-1735(2)	5393(2)	2372(1)	28(1)
C(28)	801(2)	700(2)	2289(1)	23(1)
C(29)	193(2)	-1330(2)	2212(1)	24(1)
C(30)	534(2)	-1957(2)	3038(2)	30(1)
C(31)	1141(3)	-1792(2)	1393(2)	39(1)
C(32)	-1366(2)	-1330(2)	2136(2)	29(1)
N	498(2)	-195(1)	2268(1)	29(1)

Table 69. Selected bond lengths [Å] and angles [°] for 15.

Ni-C(28)	1.864(2)	C(28)-Ni-P(1)	104.56(6)
Ni-P(1)	2.2403(5)	C(28)-Ni-P(3)	131.79(7)
Ni-P(3)	2.2562(6)	P(1)-Ni-P(3)	93.50(2)
Ni-P(2)	2.2749(6)	C(28)-Ni-P(2)	124.37(7)
Ni-B	3.431(2)	P(1)-Ni-P(2)	96.83(2)
C(28)-N	1.164(2)	P(3)-Ni-P(2)	96.42(2)
		N-C(28)-Ni	177.53(19)
		C(28)-N-C(29)	176.9(2)

Table 70. Bond lengths [Å] and angles [°] for 15.

Ni-C(28)	1.864(2)	C(17A)-H(17A)	1.0000
Ni-P(1)	2.2403(5)	C(18A)-H(18A)	0.9800
Ni-P(3)	2.2562(6)	C(18A)-H(18B)	0.9800
Ni-P(2)	2.2749(6)	C(18A)-H(18C)	0.9800
Ni-B	3.431(2)	C(17B)-C(16)	1.491(6)
P(3)-C(9)	1.8345(18)	C(17B)-C(18B)	1.525(9)
P(3)-C(23)	1.865(2)	C(17B)-H(17B)	1.0000
P(3)-C(26)	1.867(2)	C(18B)-H(18D)	0.9800
P(2)-C(8)	1.8238(19)	C(18B)-H(18E)	0.9800
P(2)-C(20)	1.871(2)	C(18B)-H(18F)	0.9800
P(2)-C(17A)	1.891(8)	C(16)-H(16A)	0.9628
P(2)-C(17B)	1.891(5)	C(16)-H(16B)	0.9807
P(1)-C(7)	1.8281(18)	C(16)-H(16C)	0.9614
P(1)-C(14)	1.865(2)	C(16)-H(16D)	0.9607
P(1)-C(11)	1.866(2)	C(16)-H(16E)	0.9711
B-C(1)	1.632(3)	C(16)-H(16F)	0.9752
B-C(7)	1.665(3)	C(19)-C(20)	1.517(2)
B-C(9)	1.674(3)	C(19)-H(19A)	0.9800
B-C(8)	1.675(3)	C(19)-H(19B)	0.9800
C(1)-C(2)	1.403(3)	C(19)-H(19C)	0.9800
C(1)-C(6)	1.406(3)	C(20)-C(21)	1.533(3)
C(2)-C(3)	1.387(3)	C(20)-H(20)	1.0000
C(2)-H(2)	0.9500	C(21)-H(21A)	0.9800
C(3)-C(4)	1.388(3)	C(21)-H(21B)	0.9800
C(3)-H(3)	0.9500	C(21)-H(21C)	0.9800
C(4)-C(5)	1.383(3)	C(22)-C(23)	1.527(3)
C(4)-H(4)	0.9500	C(22)-H(22A)	0.9800
C(5)-C(6)	1.389(3)	C(22)-H(22B)	0.9800
C(5)-H(5)	0.9500	C(22)-H(22C)	0.9800
C(6)-H(6)	0.9500	C(23)-C(24)	1.538(3)
C(7)-H(7A)	0.9900	C(23)-H(23)	1.0000
C(7)-H(7B)	0.9900	C(24)-H(24A)	0.9800
C(8)-H(8A)	0.9900	C(24)-H(24B)	0.9800
C(8)-H(8B)	0.9900	C(24)-H(24C)	0.9800
C(9)-H(9A)	0.9900	C(25)-C(26)	1.442(3)
C(9)-H(9B)	0.9900	C(25)-H(25A)	0.9800
C(10)-C(11)	1.530(3)	C(25)-H(25B)	0.9800
C(10)-H(10A)	0.9800	C(25)-H(25C)	0.9800
C(10)-H(10B)	0.9800	C(26)-C(27)	1.504(3)
C(10)-H(10C)	0.9800	C(26)-H(26)	1.0000
C(11)-C(12)	1.538(3)	C(27)-H(27A)	0.9800
C(11)-H(11)	1.0000	C(27)-H(27B)	0.9800
C(12)-H(12A)	0.9800	C(27)-H(27C)	0.9800
C(12)-H(12B)	0.9800	C(28)-N	1.164(2)
C(12)-H(12C)	0.9800	C(29)-N	1.458(3)
C(13)-C(14)	1.540(3)	C(29)-C(30)	1.524(3)
C(13)-H(13A)	0.9800	C(29)-C(32)	1.526(3)
C(13)-H(13B)	0.9800	C(29)-C(31)	1.530(3)
C(13)-H(13C)	0.9800	C(30)-H(30A)	0.9800
C(14)-C(15)	1.530(3)	C(30)-H(30B)	0.9800
C(14)-H(14)	1.0000	C(30)-H(30C)	0.9800
C(15)-H(15A)	0.9800	C(31)-H(31A)	0.9800
C(15)-H(15B)	0.9800	C(31)-H(31B)	0.9800
C(15)-H(15C)	0.9800	C(31)-H(31C)	0.9800
C(17A)-C(18A)	1.539(15)	C(32)-H(32A)	0.9800
C(17A)-C(16)	1.567(8)	C(32)-H(32B)	0.9800

C(32)-H(32C)	0.9800	C(6)-C(5)-H(5)	119.9
		C(5)-C(6)-C(1)	123.50(18)
C(28)-Ni-P(1)	104.56(6)	C(5)-C(6)-H(6)	118.2
C(28)-Ni-P(3)	131.79(7)	C(1)-C(6)-H(6)	118.2
P(1)-Ni-P(3)	93.50(2)	B-C(7)-P(1)	116.14(13)
C(28)-Ni-P(2)	124.37(7)	B-C(7)-H(7A)	108.3
P(1)-Ni-P(2)	96.83(2)	P(1)-C(7)-H(7A)	108.3
P(3)-Ni-P(2)	96.42(2)	B-C(7)-H(7B)	108.3
C(28)-Ni-B	162.66(7)	P(1)-C(7)-H(7B)	108.3
P(1)-Ni-B	58.67(4)	H(7A)-C(7)-H(7B)	107.4
P(3)-Ni-B	58.87(4)	B-C(8)-P(2)	116.69(14)
P(2)-Ni-B	58.87(4)	B-C(8)-H(8A)	108.1
C(9)-P(3)-C(23)	103.55(9)	P(2)-C(8)-H(8A)	108.1
C(9)-P(3)-C(26)	106.45(10)	B-C(8)-H(8B)	108.1
C(23)-P(3)-C(26)	107.08(11)	P(2)-C(8)-H(8B)	108.1
C(9)-P(3)-Ni	108.49(6)	H(8A)-C(8)-H(8B)	107.3
C(23)-P(3)-Ni	117.86(7)	B-C(9)-P(3)	115.95(13)
C(26)-P(3)-Ni	112.50(8)	B-C(9)-H(9A)	108.3
C(8)-P(2)-C(20)	103.21(9)	P(3)-C(9)-H(9A)	108.3
C(8)-P(2)-C(17A)	103.6(3)	B-C(9)-H(9B)	108.3
C(20)-P(2)-C(17A)	114.0(4)	P(3)-C(9)-H(9B)	108.3
C(8)-P(2)-C(17B)	109.54(19)	H(9A)-C(9)-H(9B)	107.4
C(20)-P(2)-C(17B)	94.9(3)	C(11)-C(10)-H(10A)	109.5
C(17A)-P(2)-C(17B)	19.09(19)	C(11)-C(10)-H(10B)	109.5
C(8)-P(2)-Ni	107.34(6)	H(10A)-C(10)-H(10B)	109.5
C(20)-P(2)-Ni	114.46(7)	C(11)-C(10)-H(10C)	109.5
C(17A)-P(2)-Ni	112.9(3)	H(10A)-C(10)-H(10C)	109.5
C(17B)-P(2)-Ni	125.1(2)	H(10B)-C(10)-H(10C)	109.5
C(7)-P(1)-C(14)	102.88(9)	C(10)-C(11)-C(12)	110.71(16)
C(7)-P(1)-C(11)	105.81(9)	C(10)-C(11)-P(1)	113.19(15)
C(14)-P(1)-C(11)	107.55(9)	C(12)-C(11)-P(1)	116.10(14)
C(7)-P(1)-Ni	109.48(6)	C(10)-C(11)-H(11)	105.3
C(14)-P(1)-Ni	113.54(7)	C(12)-C(11)-H(11)	105.3
C(11)-P(1)-Ni	116.46(7)	P(1)-C(11)-H(11)	105.3
C(1)-B-C(7)	109.34(15)	C(11)-C(12)-H(12A)	109.5
C(1)-B-C(9)	105.56(15)	C(11)-C(12)-H(12B)	109.5
C(7)-B-C(9)	110.07(16)	H(12A)-C(12)-H(12B)	109.5
C(1)-B-C(8)	108.66(16)	C(11)-C(12)-H(12C)	109.5
C(7)-B-C(8)	110.10(15)	H(12A)-C(12)-H(12C)	109.5
C(9)-B-C(8)	112.97(15)	H(12B)-C(12)-H(12C)	109.5
C(1)-B-Ni	177.71(13)	C(14)-C(13)-H(13A)	109.5
C(7)-B-Ni	72.43(10)	C(14)-C(13)-H(13B)	109.5
C(9)-B-Ni	72.31(10)	H(13A)-C(13)-H(13B)	109.5
C(8)-B-Ni	71.75(10)	C(14)-C(13)-H(13C)	109.5
C(2)-C(1)-C(6)	114.06(17)	H(13A)-C(13)-H(13C)	109.5
C(2)-C(1)-B	121.77(16)	H(13B)-C(13)-H(13C)	109.5
C(6)-C(1)-B	124.02(17)	C(15)-C(14)-C(13)	110.49(16)
C(3)-C(2)-C(1)	123.50(18)	C(15)-C(14)-P(1)	116.96(15)
C(3)-C(2)-H(2)	118.3	C(13)-C(14)-P(1)	112.74(15)
C(1)-C(2)-H(2)	118.3	C(15)-C(14)-H(14)	105.2
C(2)-C(3)-C(4)	120.19(18)	C(13)-C(14)-H(14)	105.2
C(2)-C(3)-H(3)	119.9	P(1)-C(14)-H(14)	105.2
C(4)-C(3)-H(3)	119.9	C(14)-C(15)-H(15A)	109.5
C(5)-C(4)-C(3)	118.57(18)	C(14)-C(15)-H(15B)	109.5
C(5)-C(4)-H(4)	120.7	H(15A)-C(15)-H(15B)	109.5
C(3)-C(4)-H(4)	120.7	C(14)-C(15)-H(15C)	109.5
C(4)-C(5)-C(6)	120.17(18)	H(15A)-C(15)-H(15C)	109.5
C(4)-C(5)-H(5)	119.9	H(15B)-C(15)-H(15C)	109.5

C(18A)-C(17A)-C(16)	116.2(8)	C(20)-C(21)-H(21A)	109.5
C(18A)-C(17A)-P(2)	114.9(7)	C(20)-C(21)-H(21B)	109.5
C(16)-C(17A)-P(2)	108.9(5)	H(21A)-C(21)-H(21B)	109.5
C(18A)-C(17A)-H(17A)	105.2	C(20)-C(21)-H(21C)	109.5
C(16)-C(17A)-H(17A)	105.2	H(21A)-C(21)-H(21C)	109.5
P(2)-C(17A)-H(17A)	105.2	H(21B)-C(21)-H(21C)	109.5
C(16)-C(17B)-C(18B)	109.2(6)	C(23)-C(22)-H(22A)	109.5
C(16)-C(17B)-P(2)	112.4(3)	C(23)-C(22)-H(22B)	109.5
C(18B)-C(17B)-P(2)	113.8(5)	H(22A)-C(22)-H(22B)	109.5
C(16)-C(17B)-H(17B)	107.0	C(23)-C(22)-H(22C)	109.5
C(18B)-C(17B)-H(17B)	107.0	H(22A)-C(22)-H(22C)	109.5
P(2)-C(17B)-H(17B)	107.0	H(22B)-C(22)-H(22C)	109.5
C(17B)-C(18B)-H(18D)	109.5	C(22)-C(23)-C(24)	109.83(17)
C(17B)-C(18B)-H(18E)	109.5	C(22)-C(23)-P(3)	112.58(15)
H(18D)-C(18B)-H(18E)	109.5	C(24)-C(23)-P(3)	116.21(14)
C(17B)-C(18B)-H(18F)	109.5	C(22)-C(23)-H(23)	105.8
H(18D)-C(18B)-H(18F)	109.5	C(24)-C(23)-H(23)	105.8
H(18E)-C(18B)-H(18F)	109.5	P(3)-C(23)-H(23)	105.8
C(17B)-C(16)-C(17A)	23.5(2)	C(23)-C(24)-H(24A)	109.5
C(17B)-C(16)-H(16A)	116.5	C(23)-C(24)-H(24B)	109.5
C(17A)-C(16)-H(16A)	111.1	H(24A)-C(24)-H(24B)	109.5
C(17B)-C(16)-H(16B)	124.7	C(23)-C(24)-H(24C)	109.5
C(17A)-C(16)-H(16B)	110.2	H(24A)-C(24)-H(24C)	109.5
H(16A)-C(16)-H(16B)	107.5	H(24B)-C(24)-H(24C)	109.5
C(17B)-C(16)-H(16C)	88.2	C(26)-C(25)-H(25A)	109.5
C(17A)-C(16)-H(16C)	111.2	C(26)-C(25)-H(25B)	109.5
H(16A)-C(16)-H(16C)	109.1	H(25A)-C(25)-H(25B)	109.5
H(16B)-C(16)-H(16C)	107.6	C(26)-C(25)-H(25C)	109.5
C(17B)-C(16)-H(16D)	111.4	H(25A)-C(25)-H(25C)	109.5
C(17A)-C(16)-H(16D)	114.6	H(25B)-C(25)-H(25C)	109.5
H(16A)-C(16)-H(16D)	19.6	C(25)-C(26)-C(27)	116.4(2)
H(16B)-C(16)-H(16D)	120.7	C(25)-C(26)-P(3)	115.10(18)
H(16C)-C(16)-H(16D)	90.5	C(27)-C(26)-P(3)	117.67(16)
C(17B)-C(16)-H(16E)	110.8	C(25)-C(26)-H(26)	101.1
C(17A)-C(16)-H(16E)	88.4	C(27)-C(26)-H(26)	101.1
H(16A)-C(16)-H(16E)	89.4	P(3)-C(26)-H(26)	101.1
H(16B)-C(16)-H(16E)	36.8	C(26)-C(27)-H(27A)	109.5
H(16C)-C(16)-H(16E)	144.5	C(26)-C(27)-H(27B)	109.5
H(16D)-C(16)-H(16E)	108.5	H(27A)-C(27)-H(27B)	109.5
C(17B)-C(16)-H(16F)	110.5	C(26)-C(27)-H(27C)	109.5
C(17A)-C(16)-H(16F)	126.5	H(27A)-C(27)-H(27C)	109.5
H(16A)-C(16)-H(16F)	119.6	H(27B)-C(27)-H(27C)	109.5
H(16B)-C(16)-H(16F)	70.5	N-C(28)-Ni	177.53(19)
H(16C)-C(16)-H(16F)	37.2	N-C(29)-C(30)	108.02(17)
H(16D)-C(16)-H(16F)	108.2	N-C(29)-C(32)	107.53(17)
H(16E)-C(16)-H(16F)	107.3	C(30)-C(29)-C(32)	112.04(18)
C(20)-C(19)-H(19A)	109.5	N-C(29)-C(31)	107.62(18)
C(20)-C(19)-H(19B)	109.5	C(30)-C(29)-C(31)	110.48(18)
H(19A)-C(19)-H(19B)	109.5	C(32)-C(29)-C(31)	110.96(17)
C(20)-C(19)-H(19C)	109.5	C(29)-C(30)-H(30A)	109.5
H(19A)-C(19)-H(19C)	109.5	C(29)-C(30)-H(30B)	109.5
H(19B)-C(19)-H(19C)	109.5	H(30A)-C(30)-H(30B)	109.5
C(19)-C(20)-C(21)	110.81(16)	C(29)-C(30)-H(30C)	109.5
C(19)-C(20)-P(2)	112.15(12)	H(30A)-C(30)-H(30C)	109.5
C(21)-C(20)-P(2)	116.39(16)	H(30B)-C(30)-H(30C)	109.5
C(19)-C(20)-H(20)	105.5	C(29)-C(31)-H(31A)	109.5
C(21)-C(20)-H(20)	105.5	C(29)-C(31)-H(31B)	109.5
P(2)-C(20)-H(20)	105.5	H(31A)-C(31)-H(31B)	109.5

C(29)-C(31)-H(31C)	109.5	H(32A)-C(32)-H(32B)	109.5
H(31A)-C(31)-H(31C)	109.5	C(29)-C(32)-H(32C)	109.5
H(31B)-C(31)-H(31C)	109.5	H(32A)-C(32)-H(32C)	109.5
C(29)-C(32)-H(32A)	109.5	H(32B)-C(32)-H(32C)	109.5
C(29)-C(32)-H(32B)	109.5	C(28)-N-C(29)	176.9(2)

Table 71. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for 15. The anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2 a^{*2} U^{11} + ... + 2\ h\ k\ a^*\ b^*\ U^{12}]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Ni	21(1)	12(1)	21(1)	-1(1)	-10(1)	-1(1)
P(3)	16(1)	14(1)	23(1)	-2(1)	-8(1)	-1(1)
P(2)	21(1)	18(1)	21(1)	-7(1)	-5(1)	-1(1)
P(1)	21(1)	11(1)	21(1)	0(1)	-10(1)	-1(1)
B	19(1)	12(1)	20(1)	0(1)	-7(1)	-1(1)
C(1)	12(1)	14(1)	23(1)	-4(1)	-4(1)	3(1)
C(2)	21(1)	16(1)	24(1)	-3(1)	-10(1)	1(1)
C(3)	26(1)	13(1)	30(1)	2(1)	-7(1)	0(1)
C(4)	22(1)	13(1)	33(1)	-5(1)	-8(1)	-3(1)
C(5)	23(1)	22(1)	24(1)	-5(1)	-8(1)	-2(1)
C(6)	20(1)	15(1)	22(1)	-1(1)	-5(1)	-1(1)
C(7)	17(1)	11(1)	22(1)	-2(1)	-8(1)	-1(1)
C(8)	18(1)	13(1)	22(1)	-1(1)	-6(1)	-1(1)
C(9)	18(1)	13(1)	16(1)	-1(1)	-6(1)	-2(1)
C(10)	48(2)	23(1)	30(1)	6(1)	-14(1)	-14(1)
C(11)	26(1)	19(1)	23(1)	2(1)	-9(1)	-3(1)
C(12)	40(1)	26(1)	24(1)	5(1)	-14(1)	-8(1)
C(13)	36(1)	16(1)	34(1)	-4(1)	-11(1)	5(1)
C(14)	22(1)	15(1)	28(1)	-2(1)	-8(1)	4(1)
C(15)	25(1)	23(1)	38(1)	-2(1)	-14(1)	6(1)
C(17A)	30(4)	20(4)	17(4)	-5(3)	-8(3)	5(3)
C(18A)	69(6)	35(6)	41(5)	-13(4)	35(5)	-14(5)
C(17B)	31(3)	23(3)	20(3)	-6(2)	-4(2)	5(2)
C(18B)	29(3)	30(3)	39(3)	-16(2)	8(2)	-4(2)
C(16)	51(2)	29(1)	37(1)	-17(1)	-15(1)	9(1)
C(19)	27	44	34	-9	-13	-1
C(20)	29(1)	33(1)	18(1)	-1(1)	-8(1)	-3(1)
C(21)	55(2)	83(2)	56(2)	45(2)	-38(2)	-34(2)
C(22)	29(1)	30(1)	31(1)	4(1)	-4(1)	-9(1)
C(23)	19(1)	24(1)	25(1)	-1(1)	-3(1)	-3(1)
C(24)	24(1)	31(1)	26(1)	-2(1)	2(1)	1(1)
C(25)	62(2)	49(2)	136(3)	35(2)	-74(2)	-26(2)
C(26)	30(1)	29(1)	62(2)	-8(1)	-32(1)	6(1)
C(27)	24(1)	30(1)	28(1)	4(1)	-8(1)	6(1)
C(28)	26(1)	19(1)	26(1)	0(1)	-10(1)	-1(1)
C(29)	26(1)	15(1)	31(1)	-5(1)	-6(1)	-5(1)
C(30)	33(1)	20(1)	39(1)	0(1)	-9(1)	-3(1)
C(31)	34(1)	42(2)	40(1)	-13(1)	1(1)	-1(1)
C(32)	26(1)	27(1)	35(1)	-5(1)	-5(1)	-4(1)
N	34(1)	21(1)	36(1)	-2(1)	-16(1)	-5(1)

Table 72. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for 15.

	x	y	z	U(eq)
H(2)	3833	6166	1760	24
H(3)	4833	7737	2020	27
H(4)	5566	7940	3372	26
H(5)	5271	6523	4447	26
H(6)	4321	4937	4165	23
H(7A)	2765	3557	4081	19
H(7B)	4341	3241	3600	19
H(8A)	4776	3396	1808	21
H(8B)	4088	4457	1352	21
H(9A)	1326	5182	2278	18
H(9B)	1167	5192	3323	18
H(10A)	2991	-285	4342	49
H(10B)	1592	-64	3909	49
H(10C)	1474	-150	4956	49
H(11)	1166	1660	4572	26
H(12A)	2457	1251	5724	43
H(12B)	2810	2405	5243	43
H(12C)	3903	1351	5048	43
H(13A)	5352	-142	2138	42
H(13B)	3761	274	2045	42
H(13C)	4077	-414	2908	42
H(14)	5050	1690	2416	26
H(15A)	5334	418	3968	42
H(15B)	5658	1680	3853	42
H(15C)	6576	798	3216	42
H(17A)	4569	1477	1052	27
H(18A)	6153	1927	-211	79
H(18B)	5919	2901	463	79
H(18C)	5164	3005	-386	79
H(17B)	3970	2749	-244	30
H(18D)	5561	1542	934	51
H(18E)	5919	2704	468	51
H(18F)	6052	1641	-109	51
H(16A)	4085	686	-247	58
H(16B)	2746	793	491	58
H(16C)	2894	1629	-317	58
H(16D)	4017	858	-406	58
H(16E)	3343	699	586	58
H(16F)	2474	1354	-69	58
H(19A)	290	3955	-207	51
H(19B)	379	2889	431	51
H(19C)	1513	2996	-451	51
H(20)	1231	4439	951	32
H(21A)	3470	4292	-513	92
H(21B)	3340	5128	265	92
H(21C)	2207	5240	-388	92
H(22A)	-1573	2513	5019	45
H(22B)	-973	1983	4089	45
H(22C)	-2382	2793	4202	45
H(23)	259	3488	4426	27
H(24A)	-2311	4757	4271	42
H(24B)	-854	5298	4256	42
H(24C)	-1543	4626	5115	42
H(25A)	-3015	3501	2868	113

H(25B)	-1926	2710	2235	113
H(25C)	-2867	3676	1823	113
H(26)	-768	4161	1688	45
H(27A)	-2219	5543	2970	42
H(27B)	-2383	5595	1955	42
H(27C)	-909	5823	2229	42
H(30A)	1540	-1930	3065	46
H(30B)	320	-2721	3020	46
H(30C)	-38	-1622	3558	46
H(31A)	936	-1361	870	58
H(31B)	958	-2557	1338	58
H(31C)	2135	-1753	1445	58
H(32A)	-1949	-994	2652	44
H(32B)	-1606	-2086	2103	44
H(32C)	-1543	-911	1603	44

Figure 13 . Fully-labeled displacement ellipsoid (50%) representation of [PhB(CH_2PPh_2)$_3$]Ni(NO) (**16**) (hydrogens omitted for clarity).

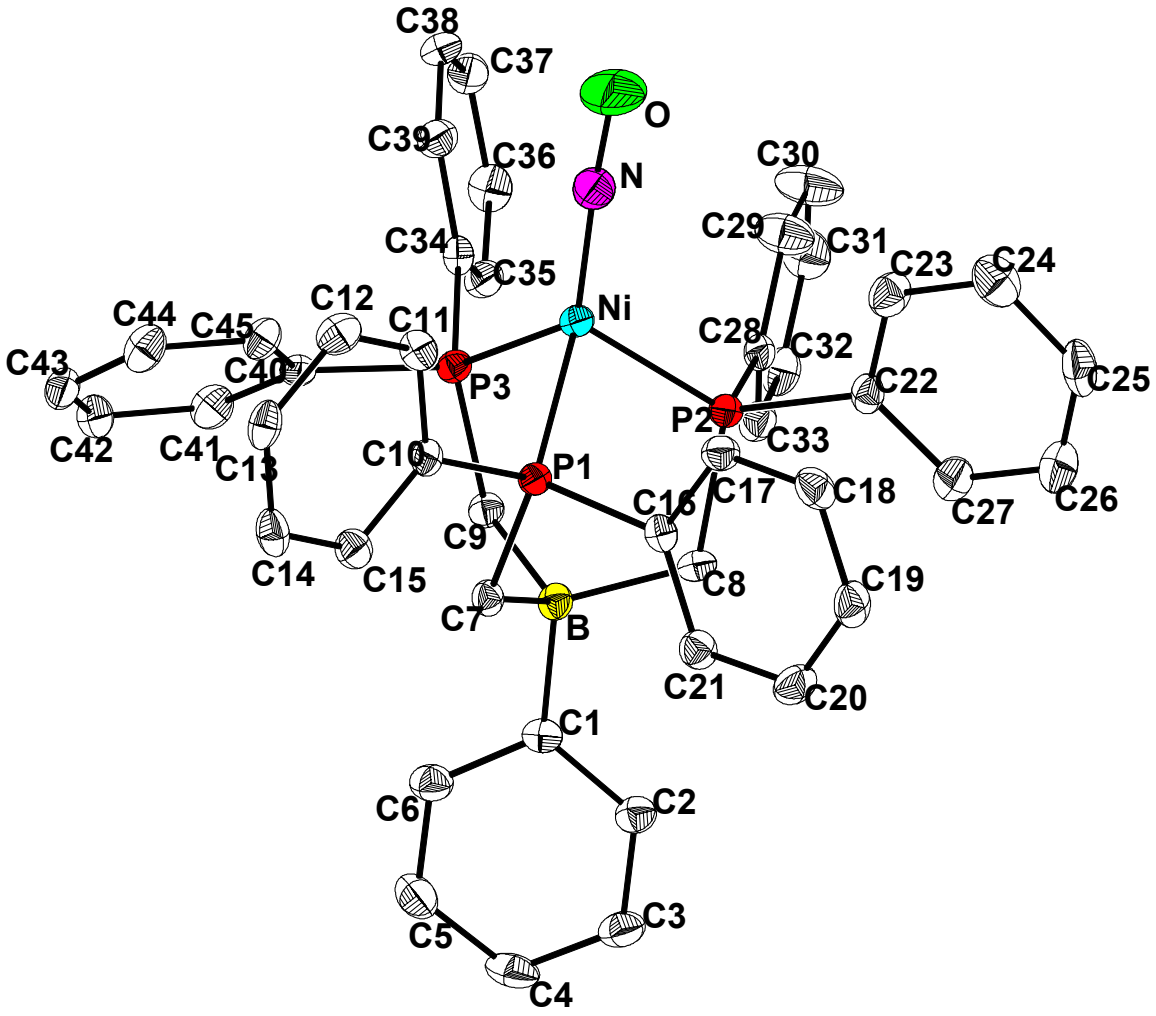


Table 73. Crystal data and structure refinement for 16.

Empirical formula	$C_{45}H_{41}BNNiOP_3$	
Moiety formula	$C_{45}H_{41}BNNiOP_3$	
Formula weight	774.22	
Crystal habit	trapezoidal	
Crystal color	red	
Crystal size	0.19 x 0.19 x 0.19 mm^3	
Data Collection		
Type of diffractometer	Bruker P4	
Wavelength	0.71073 Å	
Temperature	96(2) K	
Unit cell dimensions	a = 39.359(4) Å	α = 90°
	b = 12.9396(13) Å	β = 110.668(2)°
	c = 16.1218(16) Å	γ = 90°
Volume	7682.2(13) $Å^3$	
Z	8	
Crystal system	Monoclinic	
Space group	C2/c	
Density (calculated)	1.339 g/cm^3	
F(000)	3232	
θ range for data collection	1.67 to 28.48°	
Completeness to θ = 28.48°	90.6%	
Index ranges	$-52 \le h \le 30$, $-16 \le k \le 17$, $-18 \le l \le 20$	
Reflections collected	23382	
Independent reflections	8807 [R(int) = 0.0728]	
Absorption coefficient	0.667 mm^{-1}	
Absorption correction	None	
Structure solution and refinement		
Structure solution program	SHELXS-97 (Sheldrick, 1990)	
Primary solution method	direct methods	
Secondary solution method	difference Fourier map	
Hydrogen placement	calculated positions	
Structure refinement program	SHELXL-97 (Sheldrick, 1997)	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	8807 / 0 / 469	
Goodness-of-fit on F^2	1.110	
Final R indices [I>2σ(I)]	R1 = 0.0492, wR2 = 0.0717	
R indices (all data)	R1 = 0.0951, wR2 = 0.0788	
Type of weighting scheme used	calculated	
Weighting scheme used	$w=1/[\sigma^2(F_o^2)]$	
Max shift/error	0.009	
Average shift/error	0.002	
Largest diff. peak and hole	0.959 and -0.773 $e \cdot Å^{-3}$	

Table 74. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$ x 10^3) for 16. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
Ni	969(1)	2782(1)	3180(1)	16(1)
P(1)	890(1)	3412(1)	1835(1)	15(1)
P(2)	1297(1)	1465(1)	3004(1)	17(1)
P(3)	1467(1)	3705(1)	3884(1)	16(1)
B	1671(1)	3072(2)	2377(2)	17(1)
N	644(1)	2582(2)	3562(2)	26(1)
O	414(1)	2375(2)	3849(2)	64(1)
C(1)	1990(1)	3240(2)	1968(2)	16(1)
C(2)	2108(1)	2481(2)	1512(2)	21(1)
C(3)	2378(1)	2651(2)	1158(2)	25(1)
C(4)	2543(1)	3596(2)	1243(2)	27(1)
C(5)	2429(1)	4378(2)	1673(2)	28(1)
C(6)	2160(1)	4202(2)	2018(2)	22(1)
C(7)	1317(1)	3810(2)	1776(2)	16(1)
C(8)	1559(1)	1824(2)	2331(2)	16(1)
C(9)	1820(1)	3479(2)	3429(2)	16(1)
C(10)	562(1)	4469(2)	1449(2)	16(1)
C(11)	262(1)	4518(2)	1712(2)	19(1)
C(12)	10(1)	5302(2)	1412(2)	24(1)
C(13)	57(1)	6057(2)	854(2)	22(1)
C(14)	353(1)	6013(2)	587(2)	22(1)
C(15)	604(1)	5223(2)	880(2)	21(1)
C(16)	697(1)	2467(2)	945(2)	15(1)
C(17)	380(1)	1967(2)	907(2)	19(1)
C(18)	214(1)	1262(2)	240(2)	23(1)
C(19)	370(1)	1038(2)	-382(2)	25(1)
C(20)	684(1)	1519(2)	-353(2)	25(1)
C(21)	848(1)	2243(2)	308(2)	20(1)
C(22)	1029(1)	316(2)	2512(2)	18(1)
C(23)	709(1)	117(2)	2644(2)	25(1)
C(24)	500(1)	-741(2)	2263(2)	31(1)
C(25)	610(1)	-1395(2)	1742(2)	31(1)
C(26)	932(1)	-1205(2)	1607(2)	40(1)
C(27)	1142(1)	-360(2)	2001(2)	35(1)
C(28)	1617(1)	948(2)	4048(2)	17(1)
C(29)	1484(1)	616(2)	4688(2)	31(1)
C(30)	1713(1)	230(3)	5483(2)	41(1)
C(31)	2082(1)	195(2)	5672(2)	30(1)
C(32)	2219(1)	527(2)	5048(2)	25(1)
C(33)	1988(1)	902(2)	4232(2)	22(1)
C(34)	1641(1)	3434(2)	5074(2)	17(1)
C(35)	1989(1)	3094(2)	5546(2)	22(1)
C(36)	2095(1)	2866(2)	6447(2)	26(1)
C(37)	1851(1)	2999(2)	6877(2)	24(1)
C(38)	1503(1)	3348(2)	6416(2)	25(1)
C(39)	1399(1)	3555(2)	5527(2)	21(1)
C(40)	1401(1)	5107(2)	3844(2)	17(1)
C(41)	1694(1)	5785(2)	4194(2)	24(1)
C(42)	1642(1)	6842(2)	4110(2)	25(1)
C(43)	1301(1)	7238(2)	3692(2)	25(1)
C(44)	1008(1)	6582(2)	3375(2)	24(1)
C(45)	1060(1)	5520(2)	3458(2)	20(1)

Table 75. Selected bond lengths [Å] and angles [°] for 16.

Ni-N	1.624(3)
Ni-P(2)	2.2154(8)
Ni-P(1)	2.2326(8)
Ni-P(3)	2.2337(8)
N-O	1.183(3)
N-Ni-P(2)	119.84(9)
N-Ni-P(1)	124.68(9)
P(2)-Ni-P(1)	92.54(3)
N-Ni-P(3)	124.01(9)
P(2)-Ni-P(3)	91.74(3)
P(1)-Ni-P(3)	95.42(3)
O-N-Ni	176.0(3)

Table 76. Bond lengths [Å] and angles [°] for 16.

Ni-N	1.624(3)	C(21)-H(21)	0.9500
Ni-P(2)	2.2154(8)	C(22)-C(23)	1.373(4)
Ni-P(1)	2.2326(8)	C(22)-C(27)	1.377(4)
Ni-P(3)	2.2337(8)	C(23)-C(24)	1.389(4)
P(1)-C(7)	1.793(3)	C(23)-H(23)	0.9500
P(1)-C(10)	1.832(3)	C(24)-C(25)	1.366(4)
P(1)-C(16)	1.834(3)	C(24)-H(24)	0.9500
P(2)-C(8)	1.803(3)	C(25)-C(26)	1.382(4)
P(2)-C(28)	1.835(3)	C(25)-H(25)	0.9500
P(2)-C(22)	1.833(3)	C(26)-C(27)	1.382(4)
P(3)-C(9)	1.811(3)	C(26)-H(26)	0.9500
P(3)-C(34)	1.829(3)	C(27)-H(27)	0.9500
P(3)-C(40)	1.830(3)	C(28)-C(29)	1.379(4)
B-C(1)	1.626(4)	C(28)-C(33)	1.386(4)
B-C(8)	1.667(4)	C(29)-C(30)	1.373(4)
B-C(9)	1.672(4)	C(29)-H(29)	0.9500
B-C(7)	1.684(4)	C(30)-C(31)	1.374(4)
N-O	1.183(3)	C(30)-H(30)	0.9500
C(1)-C(2)	1.401(4)	C(31)-C(32)	1.369(4)
C(1)-C(6)	1.403(4)	C(31)-H(31)	0.9500
C(2)-C(3)	1.388(4)	C(32)-C(33)	1.396(4)
C(2)-H(2)	0.9500	C(32)-H(32)	0.9500
C(3)-C(4)	1.369(4)	C(33)-H(33)	0.9500
C(3)-H(3)	0.9500	C(34)-C(35)	1.381(3)
C(4)-C(5)	1.386(4)	C(34)-C(39)	1.399(4)
C(4)-H(4)	0.9500	C(35)-C(36)	1.394(4)
C(5)-C(6)	1.377(4)	C(35)-H(35)	0.9500
C(5)-H(5)	0.9500	C(36)-C(37)	1.377(4)
C(6)-H(6)	0.9500	C(36)-H(36)	0.9500
C(7)-H(7A)	0.9900	C(37)-C(38)	1.385(4)
C(7)-H(7B)	0.9900	C(37)-H(37)	0.9500
C(8)-H(8A)	0.9900	C(38)-C(39)	1.371(4)
C(8)-H(8B)	0.9900	C(38)-H(38)	0.9500
C(9)-H(9A)	0.9900	C(39)-H(39)	0.9500
C(9)-H(9B)	0.9900	C(40)-C(45)	1.372(3)
C(10)-C(15)	1.389(4)	C(40)-C(41)	1.400(4)
C(10)-C(11)	1.391(4)	C(41)-C(42)	1.383(4)
C(11)-C(12)	1.380(3)	C(41)-H(41)	0.9500
C(11)-H(11)	0.9500	C(42)-C(43)	1.372(4)
C(12)-C(13)	1.384(4)	C(42)-H(42)	0.9500
C(12)-H(12)	0.9500	C(43)-C(44)	1.376(4)
C(13)-C(14)	1.377(4)	C(43)-H(43)	0.9500
C(13)-H(13)	0.9500	C(44)-C(45)	1.389(3)
C(14)-C(15)	1.384(3)	C(44)-H(44)	0.9500
C(14)-H(14)	0.9500	C(45)-H(45)	0.9500
C(15)-H(15)	0.9500		
C(16)-C(21)	1.386(4)	N-Ni-P(2)	119.84(9)
C(16)-C(17)	1.385(4)	N-Ni-P(1)	124.68(9)
C(17)-C(18)	1.386(4)	P(2)-Ni-P(1)	92.54(3)
C(17)-H(17)	0.9500	N-Ni-P(3)	124.01(9)
C(18)-C(19)	1.378(4)	P(2)-Ni-P(3)	91.74(3)
C(18)-H(18)	0.9500	P(1)-Ni-P(3)	95.42(3)
C(19)-C(20)	1.371(4)	C(7)-P(1)-C(10)	109.22(12)
C(19)-H(19)	0.9500	C(7)-P(1)-C(16)	106.73(13)
C(20)-C(21)	1.394(4)	C(10)-P(1)-C(16)	100.58(11)
C(20)-H(20)	0.9500	C(7)-P(1)-Ni	110.22(9)

C(10)-P(1)-Ni	116.21(10)	C(15)-C(10)-P(1)	121.0(2)
C(16)-P(1)-Ni	113.15(9)	C(11)-C(10)-P(1)	120.3(2)
C(8)-P(2)-C(28)	106.99(13)	C(12)-C(11)-C(10)	120.6(3)
C(8)-P(2)-C(22)	108.22(13)	C(12)-C(11)-H(11)	119.7
C(28)-P(2)-C(22)	101.86(12)	C(10)-C(11)-H(11)	119.7
C(8)-P(2)-Ni	111.17(9)	C(11)-C(12)-C(13)	120.1(3)
C(28)-P(2)-Ni	113.91(9)	C(11)-C(12)-H(12)	119.9
C(22)-P(2)-Ni	114.05(10)	C(13)-C(12)-H(12)	119.9
C(9)-P(3)-C(34)	109.68(13)	C(14)-C(13)-C(12)	119.7(3)
C(9)-P(3)-C(40)	105.42(13)	C(14)-C(13)-H(13)	120.2
C(34)-P(3)-C(40)	102.90(12)	C(12)-C(13)-H(13)	120.2
C(9)-P(3)-Ni	111.66(9)	C(13)-C(14)-C(15)	120.4(3)
C(34)-P(3)-Ni	111.57(9)	C(13)-C(14)-H(14)	119.8
C(40)-P(3)-Ni	115.08(9)	C(15)-C(14)-H(14)	119.8
C(1)-B-C(8)	109.9(2)	C(14)-C(15)-C(10)	120.4(3)
C(1)-B-C(9)	108.8(2)	C(14)-C(15)-H(15)	119.8
C(8)-B-C(9)	110.0(2)	C(10)-C(15)-H(15)	119.8
C(1)-B-C(7)	106.9(2)	C(21)-C(16)-C(17)	118.9(2)
C(8)-B-C(7)	111.9(2)	C(21)-C(16)-P(1)	123.4(2)
C(9)-B-C(7)	109.2(2)	C(17)-C(16)-P(1)	117.7(2)
O-N-Ni	176.0(3)	C(18)-C(17)-C(16)	120.8(3)
C(2)-C(1)-C(6)	114.3(3)	C(18)-C(17)-H(17)	119.6
C(2)-C(1)-B	124.5(2)	C(16)-C(17)-H(17)	119.6
C(6)-C(1)-B	121.2(2)	C(19)-C(18)-C(17)	119.5(3)
C(3)-C(2)-C(1)	123.3(3)	C(19)-C(18)-H(18)	120.2
C(3)-C(2)-H(2)	118.4	C(17)-C(18)-H(18)	120.2
C(1)-C(2)-H(2)	118.4	C(20)-C(19)-C(18)	120.6(3)
C(4)-C(3)-C(2)	120.3(3)	C(20)-C(19)-H(19)	119.7
C(4)-C(3)-H(3)	119.8	C(18)-C(19)-H(19)	119.7
C(2)-C(3)-H(3)	119.8	C(19)-C(20)-C(21)	119.8(3)
C(3)-C(4)-C(5)	118.5(3)	C(19)-C(20)-H(20)	120.1
C(3)-C(4)-H(4)	120.8	C(21)-C(20)-H(20)	120.1
C(5)-C(4)-H(4)	120.8	C(16)-C(21)-C(20)	120.3(3)
C(6)-C(5)-C(4)	120.7(3)	C(16)-C(21)-H(21)	119.8
C(6)-C(5)-H(5)	119.7	C(20)-C(21)-H(21)	119.8
C(4)-C(5)-H(5)	119.7	C(23)-C(22)-C(27)	118.7(3)
C(5)-C(6)-C(1)	122.9(3)	C(23)-C(22)-P(2)	120.2(2)
C(5)-C(6)-H(6)	118.5	C(27)-C(22)-P(2)	121.1(2)
C(1)-C(6)-H(6)	118.5	C(22)-C(23)-C(24)	120.9(3)
B-C(7)-P(1)	113.96(18)	C(22)-C(23)-H(23)	119.5
B-C(7)-H(7A)	108.8	C(24)-C(23)-H(23)	119.5
P(1)-C(7)-H(7A)	108.8	C(25)-C(24)-C(23)	119.9(3)
B-C(7)-H(7B)	108.8	C(25)-C(24)-H(24)	120.0
P(1)-C(7)-H(7B)	108.8	C(23)-C(24)-H(24)	120.0
H(7A)-C(7)-H(7B)	107.7	C(24)-C(25)-C(26)	119.7(3)
B-C(8)-P(2)	114.92(19)	C(24)-C(25)-H(25)	120.2
B-C(8)-H(8A)	108.5	C(26)-C(25)-H(25)	120.2
P(2)-C(8)-H(8A)	108.5	C(25)-C(26)-C(27)	119.9(3)
B-C(8)-H(8B)	108.5	C(25)-C(26)-H(26)	120.0
P(2)-C(8)-H(8B)	108.5	C(27)-C(26)-H(26)	120.0
H(8A)-C(8)-H(8B)	107.5	C(22)-C(27)-C(26)	120.8(3)
B-C(9)-P(3)	114.59(18)	C(22)-C(27)-H(27)	119.6
B-C(9)-H(9A)	108.6	C(26)-C(27)-H(27)	119.6
P(3)-C(9)-H(9A)	108.6	C(29)-C(28)-C(33)	118.3(3)
B-C(9)-H(9B)	108.6	C(29)-C(28)-P(2)	118.8(2)
P(3)-C(9)-H(9B)	108.6	C(33)-C(28)-P(2)	122.9(2)
H(9A)-C(9)-H(9B)	107.6	C(30)-C(29)-C(28)	121.0(3)
C(15)-C(10)-C(11)	118.7(3)	C(30)-C(29)-H(29)	119.5

C(28)-C(29)-H(29)	119.5	C(39)-C(38)-C(37)	119.8(3)
C(31)-C(30)-C(29)	120.8(3)	C(39)-C(38)-H(38)	120.1
C(31)-C(30)-H(30)	119.6	C(37)-C(38)-H(38)	120.1
C(29)-C(30)-H(30)	119.6	C(38)-C(39)-C(34)	121.1(3)
C(32)-C(31)-C(30)	119.2(3)	C(38)-C(39)-H(39)	119.4
C(32)-C(31)-H(31)	120.4	C(34)-C(39)-H(39)	119.4
C(30)-C(31)-H(31)	120.4	C(45)-C(40)-C(41)	118.3(2)
C(31)-C(32)-C(33)	120.3(3)	C(45)-C(40)-P(3)	120.4(2)
C(31)-C(32)-H(32)	119.8	C(41)-C(40)-P(3)	121.3(2)
C(33)-C(32)-H(32)	119.8	C(42)-C(41)-C(40)	120.5(3)
C(28)-C(33)-C(32)	120.4(3)	C(42)-C(41)-H(41)	119.7
C(28)-C(33)-H(33)	119.8	C(40)-C(41)-H(41)	119.7
C(32)-C(33)-H(33)	119.8	C(43)-C(42)-C(41)	120.2(3)
C(35)-C(34)-C(39)	118.2(3)	C(43)-C(42)-H(42)	119.9
C(35)-C(34)-P(3)	124.8(2)	C(41)-C(42)-H(42)	119.9
C(39)-C(34)-P(3)	117.0(2)	C(42)-C(43)-C(44)	119.9(3)
C(34)-C(35)-C(36)	121.0(3)	C(42)-C(43)-H(43)	120.0
C(34)-C(35)-H(35)	119.5	C(44)-C(43)-H(43)	120.0
C(36)-C(35)-H(35)	119.5	C(43)-C(44)-C(45)	119.9(3)
C(37)-C(36)-C(35)	119.5(3)	C(43)-C(44)-H(44)	120.0
C(37)-C(36)-H(36)	120.2	C(45)-C(44)-H(44)	120.0
C(35)-C(36)-H(36)	120.2	C(40)-C(45)-C(44)	121.1(3)
C(38)-C(37)-C(36)	120.2(3)	C(40)-C(45)-H(45)	119.5
C(38)-C(37)-H(37)	119.9	C(44)-C(45)-H(45)	119.5
C(36)-C(37)-H(37)	119.9		

Table 77. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for 16. The anisotropic displacement factor exponent takes the form: $-2\pi^2[\ h^2 a^{*2} U^{11} + ... + 2\ h\ k\ a^*\ b^*\ U^{12}]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Ni	17(1)	17(1)	15(1)	0(1)	7(1)	1(1)
P(1)	16(1)	15(1)	15(1)	0(1)	6(1)	0(1)
P(2)	18(1)	16(1)	17(1)	1(1)	7(1)	1(1)
P(3)	16(1)	17(1)	15(1)	0(1)	6(1)	2(1)
B	15(2)	16(2)	19(2)	1(1)	6(1)	2(1)
N	23(2)	26(2)	30(2)	-5(1)	10(1)	-5(1)
O	65(2)	64(2)	91(2)	-19(2)	63(2)	-20(2)
C(1)	13(2)	21(2)	15(2)	3(1)	4(1)	4(1)
C(2)	20(2)	23(2)	20(2)	2(1)	8(1)	3(1)
C(3)	26(2)	29(2)	24(2)	3(1)	14(1)	7(2)
C(4)	20(2)	36(2)	29(2)	12(2)	14(1)	4(2)
C(5)	28(2)	22(2)	36(2)	6(2)	14(2)	0(2)
C(6)	21(2)	25(2)	24(2)	3(1)	11(1)	2(1)
C(7)	19(2)	14(1)	14(2)	-1(1)	4(1)	-2(1)
C(8)	15(2)	22(2)	13(2)	0(1)	5(1)	3(1)
C(9)	13(2)	16(2)	19(2)	0(1)	5(1)	2(1)
C(10)	17(2)	15(2)	15(2)	-5(1)	3(1)	-5(1)
C(11)	16(2)	19(2)	20(2)	2(1)	4(1)	1(1)
C(12)	18(2)	29(2)	23(2)	-3(1)	7(1)	2(1)
C(13)	22(2)	16(2)	20(2)	-4(1)	-2(1)	3(1)
C(14)	28(2)	14(2)	19(2)	2(1)	1(1)	-1(1)
C(15)	19(2)	19(2)	23(2)	-3(1)	7(1)	-3(1)
C(16)	14(2)	13(2)	13(2)	4(1)	0(1)	2(1)
C(17)	21(2)	20(2)	17(2)	1(1)	8(1)	1(1)
C(18)	21(2)	23(2)	25(2)	0(1)	7(1)	-7(1)
C(19)	31(2)	20(2)	19(2)	-5(1)	4(1)	-5(2)
C(20)	32(2)	27(2)	17(2)	-3(1)	9(1)	1(2)
C(21)	21(2)	19(2)	19(2)	0(1)	6(1)	-1(1)
C(22)	24(2)	14(2)	16(2)	2(1)	4(1)	3(1)
C(23)	22(2)	26(2)	25(2)	-8(1)	7(1)	-4(2)
C(24)	26(2)	33(2)	30(2)	0(2)	4(2)	-9(2)
C(25)	41(2)	17(2)	26(2)	-2(1)	2(2)	-6(2)
C(26)	62(3)	24(2)	41(2)	-10(2)	27(2)	-6(2)
C(27)	42(2)	23(2)	51(2)	-8(2)	31(2)	-5(2)
C(28)	21(2)	12(2)	18(2)	2(1)	7(1)	3(1)
C(29)	23(2)	44(2)	27(2)	13(2)	9(2)	3(2)
C(30)	40(2)	60(2)	27(2)	18(2)	16(2)	5(2)
C(31)	33(2)	31(2)	23(2)	8(2)	4(2)	5(2)
C(32)	21(2)	21(2)	29(2)	-1(1)	5(1)	7(1)
C(33)	26(2)	19(2)	22(2)	1(1)	8(1)	6(1)
C(34)	19(2)	13(2)	19(2)	-1(1)	5(1)	-1(1)
C(35)	23(2)	22(2)	23(2)	-3(1)	11(1)	0(1)
C(36)	25(2)	26(2)	23(2)	2(1)	3(1)	4(2)
C(37)	36(2)	22(2)	15(2)	2(1)	9(1)	2(2)
C(38)	35(2)	24(2)	24(2)	-5(1)	19(2)	-2(2)
C(39)	23(2)	23(2)	20(2)	-1(1)	9(1)	1(1)
C(40)	22(2)	18(2)	13(2)	1(1)	8(1)	0(1)
C(41)	20(2)	25(2)	26(2)	0(1)	7(1)	6(1)
C(42)	28(2)	19(2)	29(2)	-5(1)	12(2)	-6(1)
C(43)	39(2)	16(2)	23(2)	-1(1)	14(2)	4(2)
C(44)	24(2)	25(2)	22(2)	-1(1)	4(1)	9(2)
C(45)	20(2)	21(2)	18(2)	-5(1)	4(1)	0(1)

Table 78. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for 16.

	x	y	z	U(eq)
H(2)	1998	1818	1441	25
H(3)	2448	2108	856	30
H(4)	2731	3713	1013	32
H(5)	2538	5042	1729	33
H(6)	2087	4757	2302	27
H(7A)	1300	3795	1148	19
H(7B)	1365	4533	1985	19
H(8A)	1785	1409	2520	20
H(8B)	1419	1643	1707	20
H(9A)	1958	4128	3467	20
H(9B)	1991	2957	3800	20
H(11)	229	4008	2101	23
H(12)	-196	5323	1588	28
H(13)	-114	6604	656	26
H(14)	385	6527	200	27
H(15)	807	5196	689	25
H(17)	276	2110	1343	23
H(18)	-6	935	211	28
H(19)	259	546	-834	30
H(20)	791	1360	-783	30
H(21)	1063	2584	323	24
H(23)	630	573	3000	30
H(24)	281	-873	2365	38
H(25)	466	-1977	1475	37
H(26)	1010	-1656	1243	48
H(27)	1366	-243	1919	41
H(29)	1231	655	4578	38
H(30)	1615	-15	5907	50
H(31)	2239	-58	6228	36
H(32)	2474	503	5172	29
H(33)	2085	1126	3801	27
H(35)	2158	3015	5252	26
H(36)	2333	2619	6762	31
H(37)	1923	2851	7492	29
H(38)	1336	3444	6715	30
H(39)	1158	3785	5212	26
H(41)	1931	5517	4493	29
H(42)	1844	7296	4342	30
H(43)	1267	7964	3621	30
H(44)	771	6856	3099	29
H(45)	856	5072	3244	24